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DEVELOPMENT OF A RAPID GC/MS METHOD FOR TYPE CHARACTERIZATION OF PETROLEUM HYDROCARBONS USING A FINNIGAN 4500 GC/MS

Final Report

by

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Burlington Ontario

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EXECUTIVE SUMMARY

Following the completion of the feasibility study in Task 1 of the project, activities shifted to software development, installation and testing. These activities were undertaken to evaluate the resulting data from a Finnigan 4500 running a version of Robinson's hydrocarbon typing method. The evaluation was to focus on the repeatability and comparability of the data (particularly to data from magnetic sector mass spectrometers).

As a result of the testing and development work, a method for the analysis of hydrocarbon types is now fully implemented on the low resolution Finnigan 4500 GC/MS equipped with the Incos data system.

The Robinson software has been converted and performes effectively on the Incos. The GC sample inlet produces good precise transfer of the samples tested to-date. The overall analysis and data processing on the Finnigan 4500 produces comparable data to magnetic sector instruments using batch inlet systems. Some differences have been found between different Finnigan 4500 quadrupole systems and additional work is required to determine the precise impact of various operational settings.

SOMMAIRE EXECUTIF

Après avoir terminer l'étude de pratique dans la première tâche du projet, des activités se sont dirigees vers le développement des ordinateurs, l'installation et le testing. Ces activités ont été effectuées afin que nous puissions évaluer l'information résultant d'un Finnigan 4500 en parcourant une version d'une méthode à dactylographier hydrocarbon de Robinson. L'évaluation était de mettre au point la répétition et la comparabilité de l'information particulièrement l'information des gros spectromètres de secteur magnétiques.

Résultant du travail d'épreuve et développement, une méthode pour l'analyse des types hydrocarbon est maintenant utilisée au complet sur une résolution basse de Finnigan 4500 GC MS équipée avec une système d'information Incos.

L'ordinateur Robinson a été transformé et fonctionne effectivement sur l'Incos. L'exemplaire de la voie GC produit une copie exacte des exemplaires testés a date. L'analyse au complet et le traitement des données sur le Finnigan 4500 produisent des données comparables aux instruments de secteur magnétiques en utilisant des systèmes de bande d'entrée. Quelques différences ont été trouvées entre les différents systèmes quadrupole Finnigan 4500 et du travail supplémentaire est requis afin de pouvoir déterminer l'impact précis de diverses opérations mise en marche.

1.0 **BACKGROUND**

1.1 TASK 1- FEASIBILITY REVIEW

The feasibility review of this project was undertaken to:

1. review the currently used MS hydrocarbon typing methodologies
2. review the applications of the Robinson method
3. assess the nature of the hardware and software limitations of the Finnigan 4500 in performing the Robinson hydrocarbon typing method
4. recommend approaches to the development, implementation and testing of the Robinson hydrocarbon typing method on the Finnigan

In performing the above it was found that no significant limitations existed in either the hardware or software of the 4500 GC/MS which would preclude the successful utilization of that system for hydrocarbon typing.

Recommendations were made to proceed to acquire the IDOS source and the ASTM programs from Finnigan, to obtain a Fortran listing of the Robinson program from an existing user (if possible), modify the programs to run on the Data General computer, add connecting programs to speed the batch processing of samples on the Incos and evaluate the resulting system through a testing program. On the analysis side, recommendations were made to evaluate the cold on-column injection technique for sample introduction, with a short 3-5 metre bonded phase for separation (more like sample introduction to the MS source), mass intensity summation using existing MSDS programs and data work up using the modified Robinson method Fortran programs.

1.2 TASK 2 OBJECTIVES

The subsequent tasks of the project had the following objectives:

1. to develop a working version of the Robinson hydrocarbon typing method on the Finnigan (Data General) computer

2. to interface the Robinson method with existing MSDS and IDOS programs in such a way that the former behaved just as any other program

3. to develop the detailed analysis conditions required to perform hydrocarbon typing on naphthas and middle distillates

4. to identify the performance characteristics of the final method in terms of precision and accuracy (ie. comparability to magnetic sector data)

2.0 SOFTWARE DEVELOPMENT

A printed copy of the Fortran source code was obtained from the Research and Development Department of American Oil Co. (Whiting, Indiana) where the program originated. A printed copy of a version of the program running on a Hewlett Packard 1000 computer was also obtained from Esso Research (Sarnia, Ont.). Esso also sent a copy of this program over a modem link. We received this copy into an Apple Macintosh where the initial editing took place.

Once the integrity of the code had been verified and the obvious changes made to make the program recognizable to the Nova 4 system it was downloaded from the Macintosh to source files on the Nova 4 disk system. The second terminal port on the Nova 4 was used for this process with the Macintosh acting as a "smart" terminal emulator.

Although the function of the program was not modified in any way a large number of changes were made both to make the program operational under Super Incos and to clean up messy sections of the old Fortran.

The largest change to be made was the division of the program into a number of overlay segments which could be swapped from the disk into main memory when the particular section of program was needed. Since the program was already divided into a number of subroutines, these provided the main segment boundaries. Most of the parameters in the original subroutine call statements had to be placed in common blocks which remained in memory at all times. Since there are several large arrays of data passed back and forth, these common blocks take up a large amount of memory. Several subroutines had to be optimized to enable them to work as overlay segments. The program now runs as a series of programs, one calling the next to completion of the analysis.

The first segment of the program was responsible for the interface with the operator and the remainder of the data system and not with the actual analysis. Finnigan provides a utility with the system called **CREATE** which creates the Fortran source for most of the interface functions. This framework was used as the basis for the first segment of the program.

Inputting the data into the program also involved a significant amount of coding. The Incos stores data in a data file format. System calls are made to the operating system to open and read the required data file and the data is decoded to Fortran format as it is read in. The data file names are obtained from the system common area and conform to the standard Incos file usage.

The output formatting was changed from 14 columns for a wide printer to 7 columns for a narrow printer. The data file information is also read in and printed as documentation for the results.

A large repetitive section of code in the routine AROMAN was changed to a series of subroutine calls to the routine which is called RESOLVE. This significantly reduced the size of the segment containing this code.

A number of arithmetic IF statements in the code were modified to remove the dependance on absolute zero real numbers for correct operation. This may not have any significant effect of the operation of the program but they represented poor coding practice. In line comments were also added in a number of places to improve readability of the code.

Once all of these changes had been made (see System Documentation in Appendix A and User Manual in Appendix B), a set of known data was analysed. The software test outputs (provided in Appendix C) show the results of the analysis from Amoco and also from the current system. Analysis of these results shows no significant difference between the two data sets and confirm the integrety of the software installed on the Incos data system. The only differences which can be seen in the results are due to the Nova's tendancy to truncate instead of round to the last digit displayed. This is obvious in the average molecular weight which prints out as 0.9 even though it was verified to be 1.0. An extra digit could be printed if this truncation is annoying.

The program will produce errors and incorrect results if the sample being analyzed does not contain peaks in the series $\Sigma 78$, $\Sigma 91$, $\Sigma 104$, $\Sigma 117$, $\Sigma 130$. The subroutine SATINT (called from AROMAN) divides by these sums while calculating interference terms. The interference calculation is difficult to apply to samples containiong no aromatics.

3.0 METHODOLOGY TESTING

3.1 CALIBRATION CONDITIONS

Two basic approaches to the calibration of the GC/MS were considered for evaluation. They were:

1. direct injection of n-hexadecane
2. variable leak of n-hexadecane through the calibration gas inlet

The expected advantage of the latter procedure was that selected masses could be monitored on the scope and fine tuning of their ratios could be effected through the adjustment of quadrupole offset, ion energy or source temperature.

There were several calibration conditions which were adopted from those used in the calibration of magnetic sector instruments in Gulf Research Laboratories. The critical aspect for hydrocarbon typing is to achieve a standard fragmentation pattern of aliphatic and cyclic hydrocarbons. The fragmentation of aliphatic hydrocarbons is much more dependant on the MS conditions than is the fragmentation of aromatic compounds. Through the careful control of the fragmentation of n-hexadecane it is expected that the quadrupole mass spectra of all hydrocarbons will be virtually identical to those produced on magnetic sector MS instruments. There are four fragmentation conditions set for n-hexadecane as identified in Section 4.0 of this report.

In the evaluation of the two procedures it was found that significant difficulties existed with the use of the calibration gas inlet for the introduction of the n-hexadecane. Despite efforts to heat the calibrant and to enlarge the leak orrifice size, no significant amount of n-hexadecane entered the MS source. Temperatures up to 100° C were used without success. High temperatures using an oil bath were not evaluated. In the evaluation of the direct injection of n-hexadecane no significant prolems were encountered using either the cold on-column injector or the split-splitless injector. Elution time for the calibrant was a direct function of the temperature of the GC oven and the specific column used for analysis. Using an column temperature of 150° C and a 5 metre DB-1 column, n-hexadecane eluted in the 1-2 minute time range. With this procedure, scans were acquired, ratios were calculated, adjustments were made to the quadrupole offset, ion energy or source temperature. Following this, additional scans were acquired and the resulting ratios were re-determined. When the conditions of calibration were fully met no further adjustments were made. An example of the calibration spectrum of n-hexadecane is shown in Figure 3-1 and the difference spectrum from the library spectrum is shown in Figure 3-2.

3.2 COLUMN SELECTION

One of the considerations in the planning phase of the project concerned the method of sample introduction to the mass spectrometer. The decision was made to use the GC as an inexpensive sample introduction system (this would also permit the use of the GC/MS for other analytical tasks) and evaluate the performance of a couple of different injectors and columns.

The columns chosen were a short capillary column (5 metre x 0.3 mm DB-1 fused silica column) and a long capillary column (30 metre x 0.3 mm DB-1 fused silica column). Preliminary data on three diesel samples supplied by Shell Canada revealed that long analysis times on the order of 30 minutes) were required for these samples and there was a significant concern for what the time requirements would be for higher boiling range samples.

FIGURE 3 - 1 FINNIGAN 4500 SPECTRUM OF N-HEXADECANE

```
MID MASS SPECTRUM                                 DATA: C16STD8 #121        BASE M/Z:  57
05/28/86 11:56:00 +  0:30                         CALI: CALI2309 #3         RIC:    636928.
SAMPLE: 1UL C16 STD @ 10NG/UL
CONDS.: IT150
 #120 TO #123 SUMMED
```

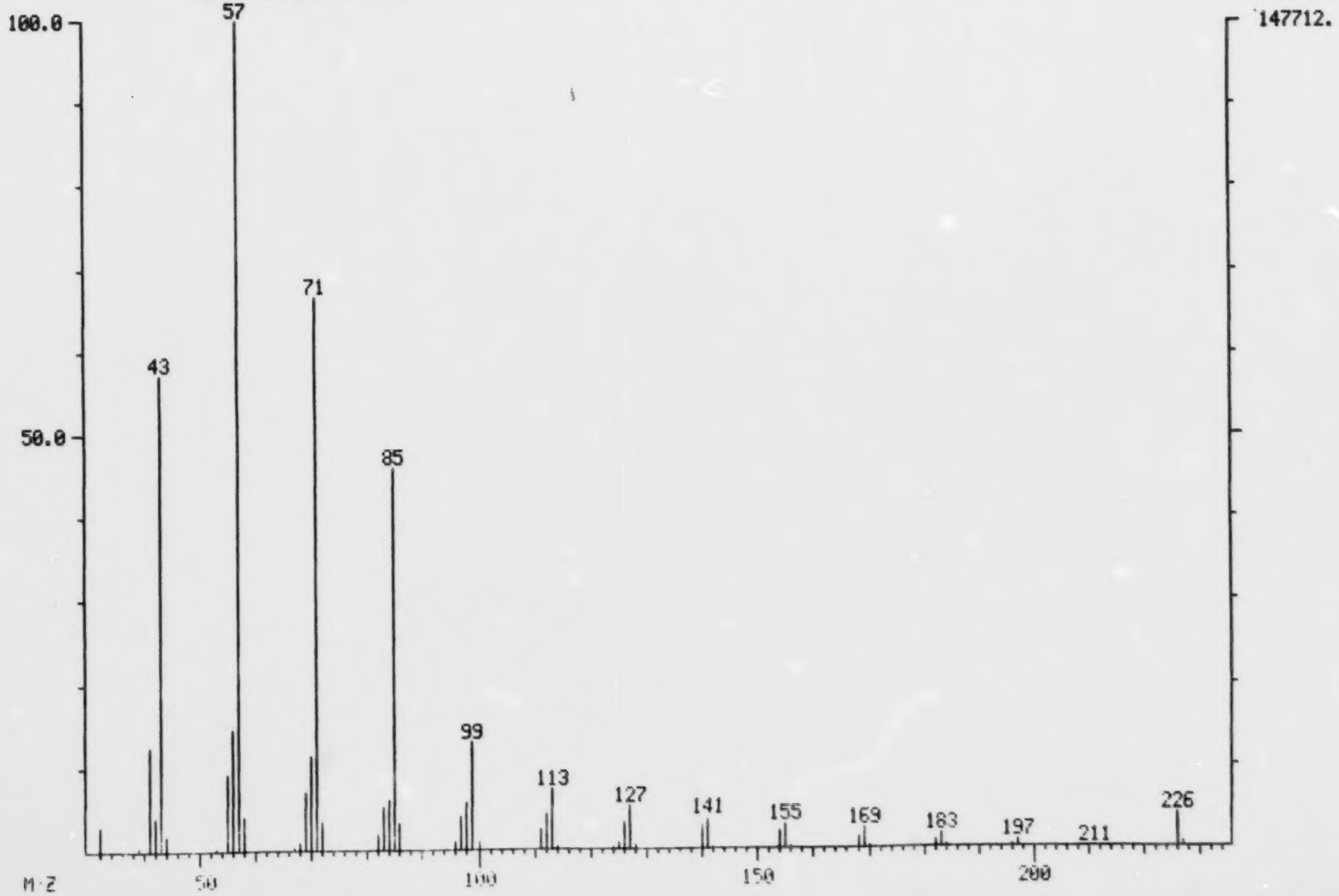
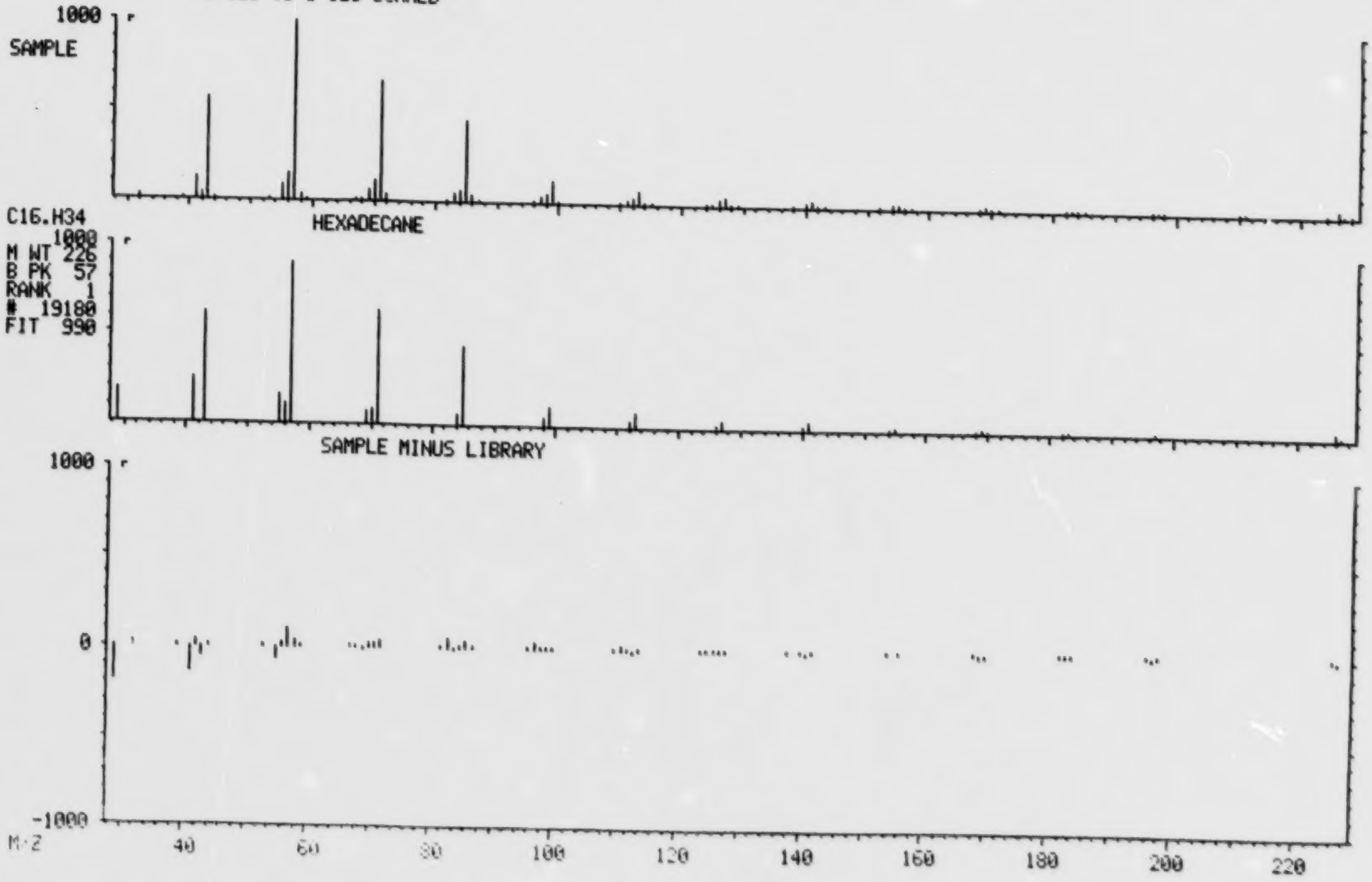


FIGURE 3 - 2 LIBRARY MATCH OF N-HEXADECANE SPECTRUM

```
MID LIBRARY SEARCH                                  DATA: C16STD8 # 121      BASE M/Z:  57
05/28/86 11:56:00 +  0:30                           CALI: CALI2309 #   3     RIC:    636927.
SAMPLE: 1UL C16 STD @ 10NG/UL
CONDS.: IT150
 # 120 TO # 123 SUMMED
```



```
C16.H34
M WT  226
B PK   57
RANK    1
#   19180
FIT   990
```

Further testing was limited to the short column and investigated the effect of column temperature on the resulting data. These tests used two samples which had been previously been analysed by magnetic sector MS systems (Gulf Research and Esso Research) using the Robinson hydrocarbon typing method. The data for both samples revealed two important results:

1. lower temperature analysis produced data much closer to the magnetic sector MS data
2. lower temperature analysis produced much more precise data on replicate injections

Examples of the low temperature and high temperature data sets on a highly aliphatic sample (sample PT-101 ; 79% saturates; 21% aromatics) are shown in Tables 3-1 and 3-2 respectively.

Under these conditions, analysis of a normal hydrocarbon standard containing from C-5 to C-40 (supplied by EMR) produced a reasonable analysis report which indicated a composition of 93.1 weight % saturates and the remainder as 5.8 weight % naphthalenes, 0.6 weight % dibenzothiophenes and 0.1 weight % naphthenebenzenes. These group overlaps are not unexpected and has been observed in other hydrocarbon typing analyses.

TABLE 3-1 LOW COLUMN TEMPERATURE TESTS ON SAMPLE PT-101

GULF - PT101
COLUMN TEMPERATURE = 150° C

All Data in Volume Percent

GROUP	Test #1	Test #2	Test #3	Test #4	Test #5	Average	Std Dev.	R.S.D.
SATURATES	71.2	68.2	69.6	69.2	67.3	69.1	1.2	1.8%
Paraffins	30.7	28.4	29.9	29.1	26.6			
Non-condensed Paraffins	21.5	20.5	20.9	20.9	20.4			
Cond. Cycloparaffins - 2 rings	12.0	10.9	11.5	11.8	11.7			
Cond. Cycloparaffins - 3 rings	7.0	8.4	7.3	7.4	8.6			
AROMATICS	27.9	30.9	29.4	30.0	31.6	30.0	1.3	4.2%
MONO-	16.8	18.7	17.1	18.0	19.1	17.9	0.9	4.8%
Benzenes	6.3	7.1	6.3	6.6	7.0			
Naphthenebenzenes	5.5	5.9	5.5	5.9	6.2			
Dinaphthenebenzenes	5.0	5.7	5.3	5.5	5.9			
DI-	8.5	9.8	9.5	9.5	9.9	9.4	0.6	6.0%
Naphthalenes	3.8	4.3	3.9	4.0	4.4			
Acenaphthenes, Dibenzofurans	2.6	2.9	2.9	2.9	3.1			
Fluorenes	2.1	2.6	2.7	2.6	2.4			
TRI-	1.3	0.9	1.4	1.2	1.2	1.2	0.2	18.0%
Phenanthrenes	1.2	0.9	1.3	1.2	1.2			
Naphthenephenanthrenes	0.1	0.0	0.1	0.0	0.0			
TETRA-	0.5	0.7	0.6	0.5	0.7	0.6	0.1	16.0%
Pyrenes	0.5	0.6	0.6	0.5	0.7			
Chrysenes	0.0	0.1	0.0	0.0	0.0			
PENTA-	0.0	0.1	0.0	0.0	0.0	0.0	0.1	250.0%
Perylenes	0.0	0.1	0.0	0.0	0.0			
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0			
THIOPHENO-	0.6	0.5	0.6	0.6	0.5	0.6	0.0	8.9%
Benzothiophenes	0.6	0.5	0.6	0.6	0.5			
Dibenzothiophenes	0.0	0.0	0.0	0.0	0.0			
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0			
UNIDENTIFIED	0.2	0.2	0.2	0.2	0.2	0.2	0.0	0.0%
Class I	0.0	0.0	0.0	0.0	0.0			
Class II	0.0	0.0	0.0	0.0	0.0			
Class III	0.0	0.0	0.0	0.0	0.0			
Class IV	0.2	0.2	0.2	0.2	0.2			
Class V	0.0	0.0	0.0	0.0	0.0			
Class VI	0.0	0.0	0.0	0.0	0.0			
Class VII	0.0	0.0	0.0	0.0	0.0			

TABLE 3-2 HIGH COLUMN TEMPERATURE TESTS ON SAMPLE PT-101

GULF - PT101
COLUMN TEMPERATURE = 300° C

All Data in Volume Percent

GROUP	Test #1	Test #2	Test #3	Test #4	Test #5	Average	Std Dev.	R.S.D.
SATURATES	44.5	44.2	32.4	49.5	45.5	43.2	7.3	16.8%
Paraffins	13.6	14.4	11.8	17.5	16.2			
Non-condensed Paraffins	12.0	12.2	9.0	13.9	12.6			
Cond. Cycloparaffins - 2 rings	7.9	7.7	5.5	8.4	7.4			
Cond. Cycloparaffins - 3 rings	11.0	9.9	6.1	9.7	9.3			
AROMATICS	54.3	54.8	66.4	49.6	53.7	55.8	7.1	12.8%
MONO-	33.2	32.2	30.8	28.7	29.7	30.9	2.0	6.3%
Benzenes	8.4	8.3	7.2	8.5	8.6			
Naphthenebenzenes	12.5	11.6	10.6	9.4	9.6			
Dinaphthenebenzenes	12.3	12.3	13.0	10.8	11.5			
DI-	16.7	16.9	24.1	16.7	18.7	18.6	3.7	19.7%
Naphthalenes	7.1	6.2	6.1	6.3	6.3			
Acenaphthenes, Dibenzofurans	3.8	4.5	7.8	4.7	5.7			
Fluorenes	5.8	6.2	10.2	5.7	6.7			
TRI-	0.6	1.5	3.2	1.1	1.5	1.6	1.1	71.4%
Phenanthrenes	0.6	1.5	2.4	1.1	1.5			
Naphthenephenanthrenes	0.0	0.0	0.8	0.0	0.0			
TETRA-	0.4	0.7	2.9	1.1	1.3	1.3	1.1	87.5%
Pyrenes	0.4	0.7	2.3	1.0	1.1			
Chrysenes	0.0	0.0	0.6	0.1	0.2			
PENTA-	0.2	0.1	0.0	0.0	0.0	0.1	0.1	159.6%
Perylenes	0.2	0.1	0.0	0.0	0.0			
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0			
THIOPHENO-	1.2	1.4	3.0	0.8	1.3	1.5	1.0	62.7%
Benzothiophenes	0.8	0.6	1.0	0.4	0.6			
Dibenzothiophenes	0.4	0.8	2.0	0.4	0.7			
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0			
UNIDENTIFIED	2.0	2.0	2.4	1.2	1.2	1.8	0.5	28.6%
Class I	0.0	0.0	0.0	0.0	0.0			
Class II	0.0	0.0	0.0	0.0	0.0			
Class III	0.0	0.0	0.0	0.0	0.0			
Class IV	0.8	1.0	1.2	0.6	0.6			
Class V	0.4	0.1	0.1	0.0	0.1			
Class VI	0.0	0.3	0.2	0.1	0.2			
Class VII	0.8	0.6	0.9	0.5	0.3			

3.3 SAMPLE INTRODUCTION

Three different sample introduction techniques were considered at the start of the project. They were:

1. solid probe introduction
2. cold on-column injection
3. split / splitless injection

All attempts to use the solid probe sample introduction were fraught with operational difficulties and were abandoned early in the study. The use of the cold on-column injector was deemed quite desireable since it is widely known that this injector produces less high mass discrimination than the split / splitless injector. Testing on the two samples supplied by Gulf and a higher boiling sample (average molecular weight = 385) supplied by Esso Canada revealed some difficulties with the procedure. The syringe and its capillary needle proved to be exceedingly difficult to clean between samples and a significant amount of sample carry over was seen into subsequent samples. In addition, there was no way to load the higher boiling (and higher viscosity) sample into the on-column syringe. These two results forced the use of the split / splitless injector for all further tests. A 1 uL injection volume was used for all samples.

3.4 DATA ACQUISITION

During the first set of tests (short column vs long column) it was found that for very low boiling samples a portion of the most volatile components was lost if the injection was made and then the acquisition was started. A technique of starting the acquisition and injecting the sample after 60 seconds was written into a procedure (EMPS) which indicated the time for injection by a series of beeps. This approach overcame the front end loss and also provides a region of the acquisition file which can be reviewed for background signals.

A test to determine the duration of the sample acquisition was developed and involved the use of a standard of dibenz(a,h)anthracene and indeno(1,2,3-cd)pyrene. The standard compounds were those with Z numbers ≥ 30 and as such were the latest eluting compounds handled by the Robinson method. (Care must be taken with some high boiling samples to ensure that no bleed materials are still eluting from the column which can adversely affect the next analysis.)

The final acquisition parameter which was found to significantly affect the processed data was the scan range. Through the inclusion of the full range from 30 to 650 Daltons it was found that erroneously high values for the tri- through penta-aromatics and the Thiopheno- groups were produced. Reduction of the scan range down to a high mass of 300 (more than sufficient to analyse the molecular ions for penta-aromatics and to include over 99% of the total ionization of all saturates contained in middle distillate samples), it was found that the data produced on the quadrupole MS much more closely approximated the magnetic sector MS data.

3.5 AINF FACTORS

Through out the testing of the program with various samples it became evident that through the selection of different AINF factors caused considerable difference in the calculated group and sub-group values. To understand the overall effects, a series of different factors were used on the two Gulf test samples. The PT-101 sample was a high saturates sample (79% saturates; 21% aromatics) and the EHTU sample was a high aromatics sample (24.5% saturates; 75.5% aromatics). The resulting data for these two samples are shown in Tables 3-3 and 3-4. Studying these results reveals that for the high saturates sample an AINF factor of 0.60 results in the minimum data difference between the quadrupole data and the magnetic sector MS data while for the high aromatics sample the best AINF factor was 0.80 (truncated in the data system to 0.798). No amount of tuning / retuning produced a situation which minimized the quadrupole and magnetic sector differences at the same AINF value. At this point in the project no further work on this parameter was possible. It was decided to complete the evaluation samples using first an average AINF factor of 0.70, reprocess the data with an AINF factor of 0.60 for samples high in saturates and an AINF factor of 0.80 for samples high in aromatics. All other samples would not be reprocessed. This reprocessing takes approximately 1-1.5 minutes per sample and is done in the **ROBINS** procedure. Only through continued testing of a wide variety of sample type will improved processing methods be developed.

TABLE 3-3 EFFECT OF AINF FACTOR ON PT-101 DATA

PT - 101 SAMPLE	Magnetic Sector	0.500	0.500 % diff	0.600	0.600 % diff	0.650	0.650 % diff	0.700	0.750	0.75
SATURATES	78.6	81.4	3.50	77.8	-1.02	76.0	-3.36	-4.29	72.5	-8.07
Paraffins	45.9	38.5	-17.54	36.8	-22.01	36.0	-24.18	-25.28	34.6	-28.07
Non-condensed Paraffins	19.3	22.3	14.42	21.4	10.32	20.8	7.48	6.52	20.4	5.54
Cond. Cycloparaffins - 2 rings	8.8	11.8	29.13	11.3	24.88	11.1	23.12	29.13	9.7	9.73
Cond. Cycloparaffins - 3 rings	4.6	8.8	62.69	8.3	57.36	8.1	55.12	45.38	7.8	51.61
AROMATICS	21.4	21.2	-0.94	21.3	-0.47	23.1	7.64	9.78	26.7	22.04
MONO-	14.0	11.1	-23.11	11.3	-21.34	12.2	-13.74	-10.53	13.9	-0.72
Benzenes	5.9	4.2	-33.66	4.4	-29.13	4.8	-20.56	-18.52	5.3	-10.71
Naphthenebenzenes	4.7	4.0	-16.09	3.9	-18.60	4.2	-11.24	-6.59	5.0	6.19
Dinaphthenebenzenes	3.4	2.9	-15.87	3.0	-12.50	3.2	-6.06	-2.99	3.6	5.71
DI-	5.9	7.8	27.74	8.2	32.62	8.8	39.46	40.54	9.8	49.68
Naphthalenes	3.1	3.8	20.29	3.9	22.86	4.2	30.14	32.43	4.7	41.03
Acenaphthenes, Dibenzofurans	1.6	2.5	43.90	2.6	47.62	2.8	54.55	54.55	3.2	66.67
Fluorenes	1.2	1.5	22.22	1.7	34.48	1.8	40.00	40.00	1.9	45.16
TRI-	0.7	0.8	13.33	0.9	25.00	0.9	25.00	25.00	1.0	35.3
Phenanthrenes	0.7	0.7	0.00	0.8	13.33	0.8	13.33	13.33	0.9	25.00
Naphthenephenanthrenes	0.0	0.1	200.00	0.1	200.00	0.1	200.00	200.00	0.1	200.00
TETRA-	0.2	0.3	40.00	0.3	40.00	0.4	66.67	66.67	0.4	66.67
Pyrenes	0.2	0.3	40.00	0.3	40.00	0.4	66.67	66.67	0.4	66.67
Chrysenes	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THIOPHENO-	0.6	1.2	66.67	0.6	0.00	0.8	28.57	28.57	1.6	90.91
Benzothiophenes	0.5	1.1	75.00	0.6	18.18	0.8	46.15	46.15	1.4	94.74
Dibenzothiophenes	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

TABLE 3-4 EFFECT OF AINF FACTOR ON EHTU DATA

EHTU Sample	Magnetic Sector	0.751	0.751 % diff.	0.798	0.798 % diff	0.850	0.850 % diff
SATURATES	25.2	29.4	15.38	25.5	1.18	21.1	-17.71
Paraffins	15.0	12.8	-15.83	11.2	-29.01	9.0	-50.00
Non-condensed Paraffins	4.4	7.8	55.74	6.8	42.86	6.1	32.38
Cond. Cycloparaffins - 2 rings	4.1	4.3	4.76	3.8	-7.59	4.7	13.64
Cond. Cycloparaffins - 3 rings	1.7	4.5	90.32	3.7	74.07	1.3	-26.67
AROMATICS	74.8	69.9	-6.77	73.8	-1.35	78.7	5.08
MONO-	49.3	38.6	-24.35	40.8	-18.87	48.1	-2.46
Benzenes	8.3	4.8	-53.44	5.1	-47.76	5.7	-37.14
Naphthenebenzenes	27.1	17.4	-43.60	18.4	-38.24	23.2	-15.51
Dinaphthenebenzenes	13.9	16.4	16.50	17.3	21.79	19.2	32.02
DI-	21.3	25.1	16.38	26.5	21.76	26.1	20.25
Naphthalenes	6.4	6.1	-4.80	6.4	0.00	7.2	11.76
Acenaphthenes, Dibenzofurans	8.2	10.2	21.74	10.8	27.37	10.4	23.66
Fluorenes	6.7	8.8	27.10	9.3	32.50	8.5	23.68
TRI-	3.0	5.0	50.00	5.3	55.42	4.1	30.99
Phenanthrenes	2.8	4.5	46.58	4.8	52.63	4.0	35.29
Naphthenephenanthrenes	0.2	0.5	85.71	0.5	85.71	0.1	-66.67
TETRA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Pyrenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chrysenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THIOPHENO-	1.2	1.2	0.00	1.2	0.00	0.4	-100.00
Benzothiophenes	0.0	0.2	200.00	0.2	200.00	0.1	200.00
Dibenzothiophenes	1.2	1.0	-18.18	1.0	-18.18	0.3	-120.00
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0

3.6 SAMPLE CONSTRAINTS

There are a few sample constraints which have been determined over the course of this project. Samples which have been fractionated or lack one or more groups of hydrocarbons may cause the Robinson method to produce divide by zero errors. This is explained more fully in Appendix B - Section 7. Samples which have high boiling ranges - into the gas oil range - will be problematic due to the increased elution time from the columnand the greater buildup of non-chromatographable materials on the head of the column. It is also expected that samples containing high concentrations of oxygenated species will produce erroneous data.

4.0 FINAL METHOD

Methodology

Set the Finnigan GC/MS to scan in the following way:

Range: 30 - 300 daltons
Time: 0.2 sec.
Delay (bottom): 0.05 sec.
Cycle time: 0.25 sec

The acquisition parameters used in the SYSTEM program are listed in Table 4-1.

1. Install appropriate GC column to split/splitless injector. Use direct connection to Mass Spectrometer.

2. Set GC temperature to operating temperature to be used for analysis.

3. Set zero of system. This is done in terms of a total system zero by switching Electron multiplier to operating voltage with conversion dynode ON and filament OFF. Watch right hand light on the Finnigan 2010 box while adjusting zero control - when it is on the point of being off then back off the zero control by one half a turn (i.e. counter clockwise). The zero can be checked and tuned more closely by acquiring background data under normal operating conditions with the filament ON. While acquiring display, the data being acquired using the following commands:

   MAP/C (V100; D1,1000; A0;E)

   This will show the data with greater sensitivity than the normal default value (V10000). The zero control can then be adjusted until an occasional signal is detected.

TABLE 4 - 1

FINNIGAN INSTRUMENT & MASS PARAMETERS

INSTRUMENT PARAMETERS:	
INTERFACE NUMBER	0
SUB-INTERFACE	0
2ND ACQU INTERFACE	-1
SUB-INTERFACE	-1
NUMBER OF ACQU BUFFERS	16
ADC SAMPLING RATE (US)	25
INSTRUMENT TYPE	0
FULL SCALE MASS	1024
ZERO SCALE MASS	1
INTENSITY/ION	2
ACQUISITION DIRECTION	UP
SAMPLES/PEAK - CENTROID	10
SAMPLES/PEAK - FRAGMENT	10
MID INSTABILITY (MMU)	0
MID OFFSET (MMU)	0
VOLTAGE SETTLING TIME(MS)	4
PEAK WIDTH (MMU)	1000
SCAN DAC (1=QUAD1 0=QUAD3)	0

MASS PARAMETERS:	
MINIMUM PEAK WIDTH	1
MIN FRAG WID AS % PEAK WID	80
BASELINE TO SUBTRACT	0
MINIMUM AREA AFTER MERGE	1
MERGE TOL AS % PEAK WIDTH	80
AREA TOL (DELTA SQRT AREA)	20
ALIGN TOL AS % PEAK WIDTH	80
MAX # OF PEAKS TO READ	2000
MASS DEF AT 100 U (MMU)	30
NOISE REJ FOR ENHA (0-4 S.D.)	2
TAIL REJ FOR ENHA (-1=NONE)	0
BKGND MULTIPLIER IN ADD	1.000
ADD OR AVERAGE IN ADD	ADD
FIRST MASS TO ADD OR ENHA	1
LAST MASS TO ADD OR ENHA	1024

4. Introduce FC43 (perfluorotributylamine) via the reference inlet. Tune the mass spectrometer using the following parameters in turn.

   QUAD OFFSET
   OFFSET PROGRAM
   LENS 3
   LENS 4
   LENS 5
   ELECTRON ENERGY

   The electron energy is particularly important as it helps control the fragmentation of the molecule.

   The ions used in the tuning process are 51 and 264. Peak shape, peak height and resolution are optimized using the various parameters in an iterative manner.

   When the tuning is complete, several scans are acquired (5) and the system is calibrated. The calibration should cover the range 31 to 293 daltons. The program FIT is then run on the calibration file as a diagnostic aid. The FIT ERROR should be less than 2% of peak width.

Gas Chromatography

5 m x 0.3 mm i.d. DB1 fused silica column
Injector Split/Splitless: Splitless - 0.5 min
Oven Temperature: 150°C isothermal
Interface Temperature: 270°C
Injection Temperature: 270°C

Mass Spectrometry

Electron Impact Ionization
Source Temp. 130° to 160° C (or as determined during calibration)
Manifold Temp. 60°C

System Checks

Control of the fragmentation of the hydrocarbon molecules is crucial to the correct assignment of the class of compound present. The fragmentation can be affected primarily by electron energy and by the source temperature and also by source cleanliness and possibly additional minor factors.

The system is checked by running a standard of hexadecane in methanol (10 ng/μL). This is analysed under the same conditions as will be used for sample analyses (see Table). The following protocol should be used:

1. Switch ON Filament
   Electron Multiplier (~1250 eV) P.Amp (10^{-7})
   Conversion Dynode
   Reamp - 10^{-7}

2. Start acquisition (acquire 500 scans) using procedure EMPS.

3. Prime syringe for a 1 μL injection.

4. At exactly 60 scans inject sample (the timing is indicated by a series of beeps, see Appendix A for details of procedures).

5. Calculate the following ratios for the hexadecane data and compare to that given in ASTM methodologies and those in use in Gulf Research as noted:

a) $\frac{\text{Intensity 127}}{\text{Intensity 226}} = 1.2 - 1.4$

b) $\frac{\Sigma\ 71}{\text{total ionization}}$ i.e. $\frac{71 + 85 + 99 + 113}{65 \text{ ---> } 227} = 0.58$

c) $\frac{71}{\text{total ionization}}$ i.e. $\frac{71}{65 \text{ ---> } 227} = 0.30 - 0.31$

d) $\frac{226}{\text{total ionization}}$ i.e. $\frac{226}{65 \text{ --->} 227} = 0.017 - 0.020$

If the ratios are not acceptable then adjust electron energy and/or source temperature, retune and recalibrate until the ratios are within the acceptable range. Our experience indicates that factors a) and d) are the most susceptible to instrument changes and should be monitored carefully. These can be adjusted; for example if ratio a) is too low then additional fragmentation should be encouraged especially if ratio d) is too high. This is accomplished by increasing electron energy. This is the first parameter which should be adjusted since it stabilizes rapidly. If the ratios can not be met by adjusting electron energy alone, then source temperature should be adjusted - increased in the above example. Approximately 30 minutes should be allowed for source temperature stabilization prior to retuning. After each adjustment a standard of hexadecane is analysed and the ratios checked.

6. When the ratios are correct, a standard which contains dibenz(a,h)anthracene and idenopyrene (10 ng each) is analysed in order to determine the length of analysis run required in order to cover the molecular weight range of interest (to 300 daltons).

7. Samples are analysed using the analysis time determined in (6).

Tuning, calibration and checking of intensity ratios of hexadecane are required on a daily basis.

Data Processing

The file names are placed into a name list as defined in the procedure being used. The appropriate procedure is then run to present:

(a) a reconstructed ion chromatogram of the sample,
(b) a summed spectrum of all the data,
(c) ROBINSON total oil output.

A series of procedures are included in Appendix A. These vary according to the run length. For example, Procedure EMR will be used to analyse runs of 3000 scans.

For ADSA to work, the scans it acts upon have to exist; it does not default to the highest scan number in the run. This implies that the delimiters for ADSA in the procedure have to be changed if runs are of different lengths. This has been incorporated into three separate procedures used for the following scan ranges: 3000, 1750, 1250. These have been found to be the most useful in terms of minimizing background contributions and including all data of interest. If the background is high, then a distortion of the class assignments can occur.

5.0 METHOD EVALUATION

5.1 PRECISION

The final methodology was tested to determine the precision or repeatability of the sample analysis and data processing package. The data for five replicate analyses on samples PT-101 and EHTU performed a single day are presented in Tables 5-1 and 5-2 respectively. These data show very good precision for all of the hydrocarbon groups present at mid to high concentrations. There is greater imprecision for those groups present at low concentrations.

A further test of the precision was to evaluate the repeatability of the analyses on the same samples on a different day. The results of these tests are presented in Tables 5-3 and 5-4 for the PT-101 sample and EHTU sample respectively. Generally there was good comparability on the saturates and aromatics group data, wiht some larger differences found for individual sub-groups. This parallels the precision data obtained within a single day's run.

5.2 ACCURACY

Measurement of accuracy generally refers to the comparability of data between a new method and the existing "standard method" . In this case the standard method is the magnetic sector MS analysis using a heated batch inlet and running a version of Robinson's hydrocarbon hyping method. With the excellent cooperation of both Gulf Research and Esso Canada, we obtained two sets of "standard method" data for the samples PT-101 and EHTU. These data and the corresponding data obtained on the Finnigan 4500 are presented in Tables 5-5 and 5-6 respectively. The 95% confidence intervals are included for both data ' sets 'and where there is no interval overlap the difference between the two is identified as significant. In both samples the overall allocation of saturates and aromatics are not significantly different for the two techniques. There are however, several significant differences for sub-groups on the PT-101 sample and for a few sub-groups on the EHTU sample.

The PT-101 sample had differences between the two data sets of 0.68% and 1.18% for the saturates and aromatics groups. Within the saturates group, differences for the sub-groups ranged from 10-60% and within the aromatics group, differences for the sub-groups ranged from 5-66%.

The EHTU sample had differences between the two data sets of 0.95% and 1.35% for the saturates and aromatics groups. Within the saturates group, differences for the sub-groups ranged from 8-74% and within the aromatics group, differences for

TABLE 5-1 PRECISION DATA FOR SAMPLE PT-101

PT - 101 SAMPLE	Magnetic Sector	All Data in Weight Percent						Aver.	Stdev.	RSD(%)
		0.598	0.598	0.598	0.598	0.598	0.598			
SATURATES	78.6	78.0	78.0	77.9	79.0	78.4	77.1	78.1	0.625	0.80
Paraffins	45.9	37.1	36.8	36.8	38.3	37.8	35.4	37.0	0.997	2.69
Non-condensed Paraffins	19.3	21.9	21.3	21.3	21.6	21.6	21.4	21.5	0.232	1.08
Cond. Cycloparaffins - 2 rings	8.8	10.4	11.5	11.4	10.7	10.5	11.3	11.0	0.489	4.45
Cond. Cycloparaffins - 3 rings	4.6	8.6	8.4	8.4	8.4	8.5	9.0	8.6	0.235	2.74
AROMATICS	21.4	21.2	21.3	21.3	20.3	20.7	22.1	21.2	0.612	2.90
MONO-	14.0	11.1	11.2	11.2	10.5	10.9	11.5	11.1	0.339	3.06
Benzenes	5.9	4.2	4.3	4.3	3.9	4.1	4.2	4.2	0.151	3.61
Naphthenebenzenes	4.7	4.0	3.9	3.9	3.8	3.9	4.2	4.0	0.138	3.49
Dinaphthenebenzenes	3.4	2.9	3.0	3.0	2.8	2.9	3.1	3.0	0.105	3.56
DI-	5.9	7.8	8.1	8.1	7.6	7.8	8.3	8.0	0.259	3.26
Naphthalenes	3.1	3.8	3.9	3.9	3.6	3.7	4.0	3.8	0.147	3.86
Acenaphthenes , Dibenzofurans	1.6	2.5	2.6	2.6	2.5	2.5	2.7	2.6	0.082	3.18
Fluorenes	1.2	1.5	1.6	1.6	1.5	1.6	1.6	1.6	0.052	3.30
TRI-	0.7	0.8	0.8	0.8	0.6	0.7	0.8	0.8	0.084	11.16
Phenanthrenes	0.7	0.7	0.7	0.7	0.6	0.6	0.7	0.7	0.052	7.75
Naphthenephenanthrenes	0.0	0.1	0.1	0.1	0.0	0.1	0.1	0.1	0.041	48.99
TETRA-	0.2	0.3	0.4	0.4	0.4	0.3	0.3	0.4	0.055	15.65
Pyrenes	0.2	0.3	0.4	0.4	0.4	0.3	0.3	0.4	0.055	15.65
Chrysenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
THIOPHENO-	0.6	1.2	0.8	0.8	1.2	1.0	1.2	1.0	0.197	19.03
Benzothiophenes	0.5	1.1	0.8	0.8	1.1	1.0	1.1	1.0	0.147	14.97
Dibenzothiophenes	0.1	0.1	0.0	0.0	0.1	0.0	0.1	0.1	0.055	109.54
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0

TABLE 5-2 PRECISION DATA FOR EHTU SAMPLE

EHTU Sample	Magnetic Sector	All Data in Weight Percen					Aver.	Stdev.	RSD(%)
		0.798	0.798	0.798	0.798	0.798			
SATURATES	25.2	24.9	25.7	24.7	25.8	26.1	25.4	0.607	2.38
Paraffins	15.0	11.0	11.2	10.7	11.5	11.5	11.2	0.342	3.06
Non-condensed Paraffins	4.4	6.7	6.9	6.6	7.0	6.6	6.8	0.182	2.69
Cond. Cycloparaffins - 2 rings	4.1	3.9	3.1	4.1	3.4	4.5	3.8	0.557	14.65
Cond. Cycloparaffins - 3 rings	1.7	3.3	4.5	3.3	3.9	3.5	3.7	0.510	13.78
AROMATICS	74.8	74.4	73.7	74.5	73.3	73.1	73.8	0.632	0.86
MONO-	49.3	43.5	39.4	43.8	35.8	41.3	40.8	3.297	8.09
Benzenes	8.3	5.8	4.8	5.9	3.7	5.3	5.1	0.897	17.59
Naphthenebenzenes	27.1	21.0	17.0	21.0	14.2	18.6	18.4	2.879	15.68
Dinaphthenebenzenes	13.9	16.7	17.6	16.9	17.9	17.4	17.3	0.495	2.86
DI-	21.3	25.6	27.3	25.7	28.3	25.4	26.5	1.278	4.83
Naphthalenes	6.4	6.9	6.4	7.0	5.6	6.2	6.4	0.567	8.84
Acenaphthenes , Dibenzofurans	8.2	10.2	11.2	10.4	11.6	10.5	10.8	0.593	5.50
Fluorenes	6.7	8.5	9.7	8.3	11.1	8.7	9.3	1.161	12.54
TRI-	3.0	4.7	5.7	4.5	6.6	5.0	5.3	0.57	16.18
Phenanthrenes	2.8	4.3	5.0	4.2	5.8	4.5	4.8	0.658	13.82
Naphthenephenanthrenes	0.2	0.4	0.7	0.3	0.8	0.5	0.5	0.207	38.40
TETRA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Pyrenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Chrysenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
THIOPHENO-	1.2	0.6	1.3	0.5	2.6	1.4	1.3	0.841	65.69
Benzothiophenes	0.0	0.2	0.3	0.1	0.4	0.2	0.2	0.114	47.51
Dibenzothiophenes	1.2	0.4	1.0	0.4	2.2	1.2	1.0	0.740	71.18
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.00
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0

TABLE 5-3 BETWEEN-DAY COMPARISON OF PT-101 DATA

		DAY 1			DAY 2		
PT-101 Sample	Magnetic Sector	Average	Stdev.	RSD(%)	Average	Stdev.	RSD(%)
SATURATES	78.6	78.1	0.63	0.80	73.9	0.36	0.49
Paraffins	45.9	37.0	1.00	2.69	38.0	0.93	2.44
Non-condensed Paraffins	19.3	21.5	0.23	1.08	16.4	0.72	4.40
Cond. Cycloparaffins - 2 rings	8.8	11.0	0.49	4.45	12.4	0.46	3.73
Cond. Cycloparaffins - 3 rings	4.6	8.6	0.24	2.73	7.1	0.35	4.88
AROMATICS	21.4	21.2	0.61	2.89	25.4	0.31	1.20
MONO-	14.0	11.2	0.34	3.03	10.4	0.25	2.41
Benzenes	5.9	4.2	0.15	3.60	3.9	0.06	1.49
Naphthenebenzenes	4.7	4.0	0.14	3.45	3.7	0.15	4.09
Dinaphthenebenzenes	3.4	3.0	0.11	3.50	2.8	0.06	2.04
DI-	5.9	8.0	0.26	3.24	10.4	0.20	1.92
Naphthalenes	3.1	3.8	0.15	3.87	4.5	0.17	3.85
Acenaphthenes, Dibenzofurans	1.6	2.6	0.08	3.15	3.6	0.00	0.00
Fluorenes	1.2	1.6	0.05	3.25	2.3	0.10	4.35
TRI-	0.7	0.8	0.08	10.50	1.7	0.06	3.33
Phenanthrenes	0.7	0.7	0.05	7.43	1.2	0.00	0.00
Naphthenephenanthrenes	0.0	0.1	0.04	41.00	0.5	0.06	10.83
TETRA-	0.2	0.4	0.06	13.75	0.9	0.29	33.31
Pyrenes	0.2	0.4	0.06	13.75	0.7	0.17	24.74
Chrysenes	0.0	0.0	0.00	0.00	0.2	0.12	69.28
PENTA-	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Perylenes	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Dibenzanthracenes	0.0	0.0	0.00	0.00	0.0	0.00	0.00
THIOPHENO-	0.6	1.1	0.20	17.91	2.0	0.10	5.00
Benzothiophenes	0.5	1.0	0.15	14.70	1.4	0.21	14.52
Dibenzothiophenes	0.1	0.1	0.06	55.00	0.6	0.29	50.94
Naphthobenzothiophenes	0.0	0.0	0.00	0.00	0.0	0.00	0.00
UNIDENTIFIED	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class I	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class II	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class III	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class IV	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class V	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class VI	0.0	0.0	0.00	0.00	0.0	0.00	0.00
Class VII	0.0	0.0	0.00	0.00	0.0	0.00	0.00

TABLE 5-4 BETWEEN-DAY COMPARISON OF EHTU SAMPLE DATA

EHTU Sample	Magnetic Sector	DAY 1			DAY 2		
		Average	Stdev.	RSD(%)	Average	Stdev.	RSD(%)
SATURATES	25.2	25.4	0.61	2.38	23.0	0.12	0.50
Paraffins	15.0	11.2	0.34	3.06	11.7	0.49	4.23
Non-condensed Paraffins	4.4	6.8	0.18	2.69	4.7	0.67	14.07
Cond. Cycloparaffins - 2 rings	4.1	3.8	0.56	14.65	3.7	0.31	8.18
Cond. Cycloparaffins - 3 rings	1.7	3.7	0.51	13.78	2.8	0.31	10.78
AROMATICS	74.8	73.8	0.63	0.86	76.4	0.06	0.08
MONO-	49.3	40.8	3.30	8.09	36.5	4.03	11.04
Benzenes	8.3	5.1	0.90	17.59	3.4	0.49	14.37
Naphthenebenzenes	27.1	18.4	2.88	15.68	13.1	3.24	24.79
Dinaphthenebenzenes	13.9	17.3	0.49	2.86	20.0	0.44	2.18
DI-	21.3	26.5	1.28	4.83	29.9	2.46	8.22
Naphthalenes	6.4	6.4	0.57	8.84	3.8	0.35	9.16
Acenaphthenes, Dibenzofurans	8.2	10.8	0.59	5.50	13.0	0.92	7.12
Fluorenes	6.7	9.3	1.16	12.54	13.1	1.84	14.01
TRI-	3.0	5.3	0.86	16.18	7.0	1.17	16.66
Phenanthrenes	2.8	4.8	0.66	13.82	6.1	0.96	15.81
Naphthenephenanthrenes	0.2	0.5	0.21	38.40	0.9	0.21	22.30
TETRA-	0.0	0.0	0.00	0	0.1	0.10	100.00
Pyrenes	0.0	0.0	0.00	0	0.1	0.10	100.00
Chrysenes	0.0	0.0	0.00	0	0.0	0.00	0.00
PENTA-	0.0	0.0	0.00	0	0.0	0.00	0.00
Perylenes	0.0	0.0	0.00	0	0.0	0.00	0.00
Dibenzanthracenes	0.0	0.0	0.00	0	0.0	0.00	0.00
THIOPHENO-	1.2	1.3	0.84	65.69	2.8	0.38	13.36
Benzothiophenes	0.0	0.2	0.11	47.51	0.4	0.00	0.00
Dibenzothiophenes	1.2	1.0	0.74	71.18	2.4	0.38	15.56
Naphthobenzothiophenes	0.0	0.0	0.00	0	0.0	0.00	0.00
UNIDENTIFIED	0.0	0.0	0.00	0	0.0	0.00	0.00
Class I	0.0	0.0	0.00	0	0.0	0.00	0.00
Class II	0.0	0.0	0.00	0	0.0	0.00	0.00
Class III	0.0	0.0	0.00	0	0.0	0.00	0.00
Class IV	0.0	0.0	0.00	0	0.0	0.00	0.00
Class V	0.0	0.0	0.00	0	0.0	0.00	0.00
Class VI	0.0	0.0	0.00	0	0.0	0.00	0.00
Class VII	0.0	0.0	0.00	0	0.0	0.00	0.00

TABLE 5-5 COMPARISON OF QUADRUPOLE AND MAGNETIC SECTOR DATA - PT-101

PT-101 Sample	Magnetic Sector ESSO	Magnetic Sector GULF	Mean	Stdev.	95% C. t value =	Int. 2.776	0.600 Mean	0.600 Stdev.	0.600 95% C. t value =	0.600 Int. 2.776	Significant Difference
SATURATES	78.6	79.4	79.0	0.6	77.4	80.6	78.1	0.625	76.4	79.8	
Paraffins	45.9	46.8	46.4	0.6	44.6	48.1	37.0	0.997	34.2	39.8	Yes
Non-condensed Paraffins	19.3	19.5	19.4	0.1	19.0	19.8	21.5	0.232	20.9	22.1	Yes
Cond. Cycloparaffins - 2 rings	8.8	10.5	9.7	1.2	6.3	13.0	11.0	0.489	9.6	12.4	
Cond. Cycloparaffins - 3 rings	4.6	2.6	3.6	1.4	0.0	7.5	8.6	0.235	7.9	9.3	Yes
AROMATICS	21.4	20.6	21.0	0.6	19.4	22.6	21.2	0.612	19.5	22.9	
MONO-	14.0	13.5	13.8	0.4	12.8	14.7	11.2	0.339	10.3	12.1	Yes
Benzenes	5.9	6.6	6.3	0.5	4.9	7.6	4.2	0.151	3.8	4.6	Yes
Naphthenebenzenes	4.7	4.2	4.5	0.4	3.5	5.4	4.0	0.138	3.6	4.4	
Dinaphthenebenzenes	3.4	2.7	3.1	0.5	1.7	4.4	3.0	0.105	2.7	3.3	
DI-	5.9	5.9	5.9	0.0	5.9	5.9	8.0	0.259	7.3	8.7	Yes
Naphthalenes	3.1	4.0	3.6	0.6	1.8	5.3	3.8	0.147	3.4	4.2	
Acenaphthenes, Dibenzofurans	1.6	0.9	1.3	0.5	0.0	2.6	2.6	0.082	2.4	2.8	Yes
Fluorenes	1.2	1.0	1.1	0.1	0.7	1.5	1.6	0.052	1.5	1.7	Yes
TRI-	0.7	0.9	0.8	0.1	0.4	1.2	0.8	0.084	0.6	1.0	
Phenanthrenes	0.7	0.7	0.7	0.0	0.7	0.7	0.7	0.052	0.6	0.8	
Naphthenephenanthrenes	0.0	0.2	0.1	0.1	0.0	0.5	0.1	0.041	0.0	0.2	
TETRA-	0.2	0.1	0.2	0.1	0.0	0.3	0.4	0.055	0.2	0.6	Yes
Pyrenes	0.2	0.1	0.2	0.1	0.0	0.3	0.4	0.055	0.2	0.6	Yes
Chrysenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
THIOPHENO-	0.6	0.1	0.4	0.3	0.0	1.3	1.1	0.197	0.6	1.6	
Benzothiophenes	0.5	0.1	0.3	0.3	0.0	1.1	1.0	0.147	0.6	1.4	
Dibenzothiophenes	0.1	0.0	0.1	0.1	0.0	0.2	0.1	0.055	0.0	0.3	
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000	0.0	0.0	

TABLE 5-6 COMPARISON OF QUADRUPOLE AND MAGNETIC SECTOR DATA - EHTU

EHTU Sample	Magnetic Sector ESSO	Magnetic Sector GULF	Mean	Stdev.	95% C. t value = 2.776	Int.	0.798 Mean	0.798 Stdev.	0.798 95% C. t value = 2.776	0.798 Int.	Significant Difference
SATURATES	25.2	23.8	24.5	1.0	21.8	27.2	25.4	0.61	23.7	27.1	
Paraffins	15.0	14.0	14.5	0.7	12.5	16.5	11.2	0.34	10.3	12.1	Yes
Non-condensed Paraffins	4.4	4.8	4.6	0.3	3.8	5.4	6.8	0.18	6.3	7.3	Yes
Cond. Cycloparaffins - 2 rings	4.1	4.7	4.4	0.4	3.2	5.6	3.8	0.56	2.3	5.3	
Cond. Cycloparaffins - 3 rings	1.7	0.3	1.0	1.0	0.0	3.7	3.7	0.51	2.3	5.1	
AROMATICS	74.8	76.2	75.5	1.0	72.8	78.2	73.8	0.63	72.0	75.6	
MONO-	49.3	55.1	52.2	4.1	40.8	63.6	40.8	3.30	31.6	50.0	
Benzenes	8.3	11.1	9.7	2.0	4.2	15.2	5.1	0.90	2.6	7.6	
Naphthenebenzenes	27.1	32.5	29.8	3.8	19.2	40.4	18.4	2.88	10.4	26.4	
Dinaphthenebenzenes	13.9	11.5	12.7	1.7	8.0	17.4	17.3	0.50	15.9	18.7	
DI-	21.3	17.5	19.4	2.7	11.9	26.9	26.5	1.28	23.0	30.0	
Naphthalenes	6.4	5.8	6.1	0.4	4.9	7.3	6.4	0.57	4.8	8.0	
Acenaphthenes, Dibenzofurans	8.2	6.6	7.4	1.1	4.3	10.5	10.8	0.59	9.2	12.4	
Fluorenes	6.7	5.2	6.0	1.1	3.0	8.9	9.3	1.16	6.1	12.5	
TRI-	3.0	2.9	3.0	0.1	2.8	3.1	5.3	0.86	2.9	7.7	
Phenanthrenes	2.8	2.9	2.9	0.1	2.7	3.0	4.8	0.66	3.0	6.6	Yes
Naphthenephenanthrenes	0.2	0.0	0.1	0.1	0.0	0.5	0.5	0.21	-0.1	1.1	
TETRA-	0.0	0.1	0.1	0.1	0.0	0.2	0.0	0.00	0.0	0.0	
Pyrenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Chrysenes	0.0	0.1	0.1	0.1	0.0	0.2	0.0	0.00	0.0	0.0	
PENTA-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Perylenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
THIOPHENO-	1.2	0.7	1.0	0.4	0.0	1.9	1.2	0.84	0.0	3.5	
Benzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.11	0.0	0.5	
Dibenzothiophenes	1.2	0.7	1.0	0.4	0.0	1.9	1.0	0.74	0.0	3.1	
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class I	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class II	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class III	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class IV	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class V	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class VI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	
Class VII	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	

the sub-groups ranged from 0.3-55% except for a couple of data points which are below 1.0 weight %.

It is intersting to note that similar differences exist within the magnetic sector data set. Examples of this are seen in the data for condensed 3-ring cycloparaffins (Esso - 4.6% ; Gulf 2.6%) and dibenzothiophenes (Esso - 0.5% ; Gulf 0.1%) in the PT-101 sample and for condensed 3-ring cycloparaffins (Esso - 1.7% ; Gulf 0.3%) and dibenzothiophenes (Esso - 1.2% ; Gulf 0.7%) in the EHTU sample. .

The other information on accuracy was mentioned previously inthat the analysis of a standard on n-paraffins resulted in an analysis report of 93.1% saturates and the remainder as 5.8 weight % naphthalenes, 0.6 weight % dibenzothiophenes and 0.1 weight % naphthenebenzenes. This analysis was within 6% of the "true"value for this sample.

5.3 EVALUATION SAMPLES

As part of the final method testing two series of evaluation samples were provided for blind analysis using the Finnigan 4500 - Robinson hydrocarbon typing methods. The resulting data for the two batches of samples are reported in Tables 5-7 and 5-8. Interpretation of these data will be performed by the Scientific Authority. It should be noted that the AINF factors were employed as outlined in Section 3.5.

5.4 EMR EVALUATION

Following the transfer of the software programs and draft final project report to the Scientific Authority, several further tests on the method were performed in the Canmet laboratories by EMR scientists. These tests involved the re-analysis of three of the above referenced evaluation samples. The resulting data were compared to previous data obtained from magnetic sector instrumentation in Gulf/Petro-Canada laboratories. Tables 5-9 to 5-11 contain the results from the tests and a comparison with the magnetic sector data.

It was quite apparent that the data obtained in the EMR laboratories were in good agreement with the magnetic sector data, very much better agreement than the data recorded in Zenon's analyses. In subsequent discussions between the two laboratories, no significant variations in the analysis conditions used were identified. It is apparent that some operating conditions have a significant impact on the method results and further study is required to fully define their exact nature.

TABLE 5-7 EMR EVALUATION SAMPLE DATA - BATCH ONE

EMR TEST SAMPLES	Sample Test #1		Sample Test #2		Sample Test #3		Sample Test #4	
	Average	Stdev.	Average	Stdev.	Average	Stdev.	Average	Stdev.
SATURATES	56.7	0.46	53.6	0.15	43.0	0.35	12.9	0.59
Paraffins	16.5	0.53	15.0	0.32	15.4	1.19	7.3	0.80
Non-condensed Paraffins	17.0	0.81	18.0	0.15	11.7	2.60	3.2	0.42
Cond. Cycloparaffins - 2 rings	13.0	0.49	12.7	0.31	7.8	2.61	1.8	0.25
Cond. Cycloparaffins - 3 rings	10.1	0.55	7.9	0.10	8.0	0.99	0.6	0.10
AROMATICS	42.4	0.44	45.5	0.12	56.1	0.35	86.5	0.60
MONO-	22.8	0.10	28.6	0.12	14.2	0.10	4.9	1.01
Benzenes	6.5	0.12	9.2	0.15	4.6	0.00	0.9	0.59
Naphthenebenzenes	8.9	0.06	11.4	0.06	5.2	0.06	2.2	0.31
Dinaphthenebenzenes	7.4	0.00	8.0	0.12	4.4	0.15	1.7	0.26
DI-	12.9	0.26	12.9	0.10	22.3	0.10	46.2	4.74
Naphthalenes	3.3	0.06	3.7	0.12	5.8	0.32	14.7	2.87
Acenaphthenes, Dibenzofurans	5.1	0.15	5.4	0.06	8.6	0.30	17.9	2.41
Fluorenes	4.5	0.10	3.8	0.10	7.9	0.06	13.7	0.57
TRI-	3.2	0.06	1.4	0.06	10.9	0.45	22.5	3.48
Phenanthrenes	2.4	0.12	1.2	0.00	9.5	0.60	21.0	2.76
Naphthenephenanthrenes	0.9	0.06	0.2	0.06	1.4	0.15	1.5	0.72
TETRA-	0.7	0.06	0.5	0.00	1.6	0.25	1.1	0.46
Pyrenes	0.6	0.00	0.5	0.00	1.2	0.35	1.1	0.46
Chrysenes	0.1	0.06	0.0	0.00	0.3	0.12	0.0	0.00
PENTA-	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Perylenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Dibenzanthracenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
THIOPHENO-	2.8	0.00	2.0	0.26	7.2	0.26	11.7	2.20
Benzothiophenes	1.9	0.10	1.8	0.12	1.6	0.10	2.7	0.25
Dibenzothiophenes	0.9	0.06	0.2	0.15	5.4	0.40	8.9	1.75
Naphthobenzothiophenes	0.0	0.06	0.0	0.00	0.2	0.21	0.2	0.20
UNIDENTIFIED	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class I	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class II	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class III	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class IV	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class V	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class VI	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class VII	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00

TABLE 5-7 EMR EVALUATION SAMPLE DATA - BATCH ONE

EMR TEST SAMPLES	Sample Test #5		Sample Test #6		Sample Test #11	
	Average	Stdev.	Average	Stdev.	Average	Stdev.
SATURATES	53.9	0.20	51.4	0.74	85.0	0.12
Paraffins	16.7	0.59	7.2	0.70	14.7	0.49
Non-condensed Paraffins	15.4	0.25	16.0	0.84	33.5	0.95
Cond. Cycloparaffins - 2 rings	12.1	0.87	16.4	1.33	23.7	0.12
Cond. Cycloparaffins - 3 rings	9.6	0.23	11.9	0.70	13.0	0.36
AROMATICS	45.1	0.06	47.6	0.62	14.2	0.15
MONO-	18.0	0.06	17.1	0.26	3.7	0.12
Benzenes	5.4	0.15	2.7	0.21	0.0	0.00
Naphthenebenzenes	5.4	0.21	5.8	0.15	0.7	0.06
Dinaphthenebenzenes	7.2	0.06	8.6	0.10	3.1	0.06
DI-	16.8	0.06	17.2	0.31	6.1	0.12
Naphthalenes	6.8	0.06	4.8	0.06	0.2	0.06
Acenaphthenes, Dibenzofurans	5.4	0.10	6.3	0.00	1.5	0.06
Fluorenes	4.7	0.15	6.1	0.26	4.3	0.00
TRI-	3.5	0.17	4.6	0.35	3.0	0.10
Phenanthrenes	2.7	0.10	3.5	0.26	2.8	0.10
Naphthenephenanthrenes	0.8	0.10	1.1	0.10	0.2	0.00
TETRA-	1.0	0.12	1.5	0.06	0.6	0.06
Pyrenes	0.9	0.06	1.3	0.06	0.6	0.06
Chrysenes	0.1	0.10	0.2	0.00	0.0	0.00
PENTA-	0.0	0.00	0.0	0.00	0.0	0.00
Perylenes	0.0	0.00	0.0	0.00	0.0	0.00
Dibenzanthracenes	0.0	0.00	0.0	0.00	0.0	0.00
THIOPHENO-	5.8	0.17	7.2	0.36	0.7	0.12
Benzothiophenes	4.1	0.17	5.8	0.20	0.4	0.00
Dibenzothiophenes	1.7	0.00	1.4	0.12	0.3	0.06
Naphthobenzothiophenes	0.0	0.00	0.0	0.06	0.1	0.06
UNIDENTIFIED	0.0	0.00	0.0	0.00	0.0	0.00
Class I	0.0	0.00	0.0	0.00	0.0	0.00
Class II	0.0	0.00	0.0	0.00	0.0	0.00
Class III	0.0	0.00	0.0	0.00	0.0	0.00
Class IV	0.0	0.00	0.0	0.00	0.0	0.00
Class V	0.0	0.00	0.0	0.00	0.0	0.00
Class VI	0.0	0.00	0.0	0.00	0.0	0.00
Class VII	0.0	0.00	0.0	0.00	0.0	0.00

TABLE 5-8 EMR EVALUATION SAMPLE DATA - BATCH TWO

EMR TEST SAMPLES	MB-499 -141		MB-499 -143		MB-499 -145		MB-499 -178	
	Average	Stdev.	Average	Stdev.	Average	Stdev.	Average	Stdev.
SATURATES	89.7	0.06	84.9	0.46	84.9	1.64	85.7	2.14
Paraffins	15.9	0.74	15.4	0.56	15.1	0.84	16.0	0.44
Non-condensed Paraffins	31.7	0.32	28.8	0.31	27.8	1.87	29.2	0.70
Cond. Cycloparaffins - 2 rings	27.7	0.29	25.6	0.00	27.5	3.08	26.1	1.71
Cond. Cycloparaffins - 3 rings	14.4	0.50	15.1	0.31	14.4	1.56	14.4	0.47
AROMATICS	9.5	0.23	14.3	0.59	14.2	1.58	13.6	2.02
MONO-	2.5	0.06	5.9	0.32	4.9	0.66	4.9	0.40
Benzenes	0.0	0.00	0.3	0.26	0.0	0.00	0.0	0.06
Naphthenebenzenes	0.8	0.06	2.6	0.06	2.0	0.58	2.1	0.00
Dinaphthenebenzenes	1.7	0.00	3.1	0.06	2.9	0.25	2.8	0.35
DI-	4.1	0.06	3.9	0.35	4.6	0.49	3.8	0.78
Naphthalenes	0.2	0.00	0.1	0.06	0.2	0.12	0.0	0.00
Acenaphthenes, Dibenzofurans	1.1	0.00	1.1	0.10	1.3	0.21	0.9	0.15
Fluorenes	2.8	0.06	2.7	0.21	3.0	0.20	2.9	0.64
TRI-	2.2	0.12	2.4	0.00	2.8	0.29	2.6	0.49
Phenanthrenes	2.1	0.12	1.8	0.06	2.2	0.21	2.1	0.35
Naphthenephenanthrenes	0.1	0.00	0.6	0.06	0.6	0.10	0.5	0.15
TETRA-	0.4	0.06	0.4	0.06	0.6	0.12	0.4	0.06
Pyrenes	0.4	0.06	0.4	0.06	0.6	0.12	0.4	0.06
Chrysenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
PENTA-	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Perylenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Dibenzanthracenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
THIOPHENO-	0.3	0.06	1.7	0.21	1.4	0.15	1.8	0.29
Benzothiophenes	0.3	0.06	1.5	0.20	1.2	0.15	1.6	0.17
Dibenzothiophenes	0.1	0.06	0.2	0.06	0.1	0.06	0.2	0.12
Naphthobenzothiophenes	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
UNIDENTIFIED	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class I	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class II	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class III	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class IV	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class V	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class VI	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Class VII	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00

TABLE 5-8 EMR EVALUATION SAMPLE DATA - BATCH TWO

EHTU SAMPLES	Sample A	Sample B	Sample C	Average	Stdev.
SATURATES	87.0	86.8	83.2	85.7	2.14
Paraffins	15.7	16.5	15.8	16.0	0.44
Non-condensed Paraffins	29.9	28.5	29.3	29.2	0.70
Cond. Cycloparaffins - 2 rings	27.2	26.9	24.1	26.1	1.71
Cond. Cycloparaffins - 3 rings	14.2	14.9	14.0	14.4	0.47
AROMATICS	12.3	12.5	15.9	13.6	2.02
MONO-	4.7	4.7	5.4	4.9	0.40
Benzenes	0.0	0.0	0.1	0.0	0.06
Naphthenebenzenes	2.1	2.1	2.1	2.1	0.00
Dinaphthenebenzenes	2.6	2.6	3.2	2.8	0.35
DI-	3.3	3.4	4.7	3.8	0.78
Naphthalenes	0.0	0.0	0.0	0.0	0.00
Acenaphthenes, Dibenzofurans	0.8	0.9	1.1	0.9	0.15
Fluorenes	2.5	2.5	3.6	2.9	0.64
TRI-	2.3	2.4	3.2	2.6	0.49
Phenanthrenes	1.9	1.9	2.5	2.1	0.35
Naphthenephenanthrenes	0.4	0.5	0.7	0.5	0.15
TETRA-	0.4	0.4	0.5	0.4	0.06
Pyrenes	0.4	0.4	0.5	0.4	0.06
Chrysenes	0.0	0.0	0.0	0.0	0.00
PENTA-	0.0	0.0	0.0	0.0	0.00
Perylenes	0.0	0.0	0.0	0.0	0.00
Dibenzanthracenes	0.0	0.0	0.0	0.0	0.00
THIOPHENO-	1.6	1.6	2.1	1.8	0.29
Benzothiophenes	1.5	1.5	1.8	1.6	0.17
Dibenzothiophenes	0.1	0.1	0.3	0.2	0.12
Naphthobenzothiophenes	0.0	0.0	0.0	0.0	0.00
UNIDENTIFIED	0.0	0.0	0.0	0.0	0.00
Class I	0.0	0.0	0.0	0.0	0.00
Class II	0.0	0.0	0.0	0.0	0.00
Class III	0.0	0.0	0.0	0.0	0.00
Class IV	0.0	0.0	0.0	0.0	0.00
Class V	0.0	0.0	0.0	0.0	0.00
Class VI	0.0	0.0	0.0	0.0	0.00
Class VII	0.0	0.0	0.0	0.0	0.00

TABLE 5-9 EMR-Gulf Data Comparison on Test Sample #1

	All Data in Volume Percent		
GROUP	EMR Analysis	Gulf Analysis	% Difference
SATURATES	72.2	75.3	4.2%
Paraffins	19.7	26.4	29.1%
Non-condensed Paraffins	24.5	24.5	0.0%
Cond. Cycloparaffins - 2 rings	17.4	16.8	3.5%
Cond. Cycloparaffins - 3 rings	10.6	7.6	33.0%
AROMATICS	27.3	24.6	10.4%
MONO-	24.7	22.4	9.8%
Benzenes	11.5	11.3	1.8%
Naphthenebenzenes	9.1	8.7	4.5%
Dinaphthenebenzenes	4.1	2.4	52.3%
DI-	2.4	2.2	8.7%
Naphthalenes	1.8	1.6	11.8%
Acenaphthenes , Dibenzofurans	0.0	0.1	200.0%
Fluorenes	0.6	0.5	18.2%
TRI-	0.0	0.0	0.0
Phenanthrenes	0.0	0.0	0.0
Naphthenephenanthrenes	0.0	0.0	0.0
TETRA-	0.2	0.0	200.0%
Pyrenes	0.0	0.0	0.0
Chrysenes	0.2	0.0	200.0%
PENTA-	0.0	0.0	0.0
Perylenes	0.0	0.0	0.0
Dibenzanthracenes	0.0	0.0	0.0
THIOPHENO-	0.0	0.0	0.0
Benzothiophenes	0.0	0.0	0.0
Dibenzothiophenes	0.0	0.0	0.0
Naphthobenzothiophenes	0.0	0.0	0.0
UNIDENTIFIED	0.0	0.0	0.0
Class I	0.0	0.0	0.0
Class II	0.0	0.0	0.0
Class III	0.0	0.0	0.0
Class IV	0.0	0.0	0.0
Class V	0.0	0.0	0.0
Class VI	0.0	0.0	0.0
Class VII	0.0	0.0	0.0

TABLE 5-10 EMR-Gulf Data Comparison on Test Sample #4

	All Data in Volume Percent		
GROUP	EMR Analysis	Gulf Analysis	% Difference
SATURATES	23.5	24.5	4.2%
Paraffins	9.0	14.6	47.5%
Non-condensed Paraffins	5.0	6.0	18.2%
Cond. Cycloparaffins - 2 rings	4.2	2.5	50.7%
Cond. Cycloparaffins - 3 rings	5.3	1.4	116.4%
AROMATICS	75.7	75.4	0.4%
MONO-	29.0	26.3	9.8%
Benzenes	12.7	12.3	3.2%
Naphthenebenzenes	12.7	11.6	9.1%
Dinaphthenebenzenes	3.6	2.4	40.0%
DI-	35.7	33.6	6.1%
Naphthalenes	24.9	22.4	10.6%
Acenaphthenes , Dibenzofurans	5.7	6.2	8.4%
Fluorenes	5.1	5.0	2.0%
TRI-	5.7	8.3	37.1%
Phenanthrenes	5.7	7.6	28.6%
Naphthenephenanthrenes	0.0	0.7	200.0%
TETRA-	0.3	2.2	152.0%
Pyrenes	0.3	2.0	147.8%
Chrysenes	0.0	0.2	200.0%
PENTA-	0.0	0.0	0.0%
Perylenes	0.0	0.0	0.0%
Dibenzanthracenes	0.0	0.0	0.0%
THIOPHENO-	3.7	5.0	29.9%
Benzothiophenes	3.7	1.9	64.3%
Dibenzothiophenes	0.0	3.1	200.0%
Naphthobenzothiophenes	0.0	0.0	0.0%
UNIDENTIFIED	1.3	0.0	200.0%
Class I	0.0	0.0	0.0%
Class II	0.0	0.0	0.0%
Class III	1.3	0.0	200.0%
Class IV	0.0	0.0	0.0%
Class V	0.0	0.0	0.0%
Class VI	0.0	0.0	0.0%
Class VII	0.0	0.0	0.0%

TABLE 5-11 EMR-Gulf Data Comparison on Test Sample #11

GROUP	EMR Analysis	Gulf Analysis	% Difference
	All Data in Volume Percent		
SATURATES	96.1	96.5	0.4%
Paraffins	15.8	16.9	6.7%
Non-condensed Paraffins	35.6	35.2	1.1%
Cond. Cycloparaffins - 2 rings	29.3	29.5	0.7%
Cond. Cycloparaffins - 3 rings	15.4	14.9	3.3%
AROMATICS	3.5	3.5	0.0%
MONO-	2.2	1.1	66.7%
Benzenes	0.0	0.0	0.0%
Naphthenebenzenes	0.8	0.0	200.0%
Dinaphthenebenzenes	1.4	1.1	24.0%
DI-	0.6	1.3	73.7%
Naphthalenes	0.6	0.4	40.0%
Acenaphthenes , Dibenzofurans	0.0	0.0	0.0%
Fluorenes	0.0	0.9	200.0%
TRI-	0.0	0.5	200.0%
Phenanthrenes	0.0	0.5	200.0%
Naphthenephenanthrenes	0.0	0.0	0.0%
TETRA-	0.7	0.6	15.4%
Pyrenes	0.2	0.6	100.0%
Chrysenes	0.5	0.0	200.0%
PENTA-	0.0	0.0	0.0%
Perylenes	0.0	0.0	0.0%
Dibenzanthracenes	0.0	0.0	0.0%
THIOPHENO-	0.0	0.0	0.0%
Benzothiophenes	0.0	0.0	0.0%
Dibenzothiophenes	0.0	0.0	0.0%
Naphthobenzothiophenes	0.0	0.0	0.0%
UNIDENTIFIED	0.0	0.0	0.0%
Class I	0.0	0.0	0.0%
Class II	0.0	0.0	0.0%
Class III	0.0	0.0	0.0%
Class IV	0.0	0.0	0.0%
Class V	0.0	0.0	0.0%
Class VI	0.0	0.0	0.0%
Class VII	0.0	0.0	0.0%

6.0 CONCLUSIONS AND RECOMMENDATIONS

There are a few conclusions that can be made on the basis of the results to-date.

1. The Robinson method software has been converted to perform effectively on the Finnigan Incos (Data General) data system.

2. The replicate analysis of many samples has shown that the use of the capillary GC as a sample inlet, is a precise technique for sample introduction to the mass spectrometer.

3. There is good comparability of data generated on the Finnigan 4500 with the data generated on magnetic sector MS instruments. This is a further indication that the capillary GC inlet is not causing significant discrimination (compared to the batch inlet system) of the high mass portions (of the samples analysed to date).

4. Through careful control of the Finnigan 4500 mass spectrometer conditions it is possible to produce comparable spectra for paraffins and cycloparaffins.

5. It is possible to process on the order of 30 samples a day through this analysis.

There are still some concerns over the differences observed between the quadrupole and magnetic sector results for some of the sub-groups. In addition, differences have been identified between two Finnigan 4500 GC/MS systems; one of which showed excellent comparability with magnetic sector data. Further work is needed to further identify the specific operating conditions which are significantly impacting the low resolution data.

7.0 ACKNOWLEDGEMENTS

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APPENDIX A

SOFTWARE DOCUMENTATION

ROBINSON'S METHOD FOR HYDROCARBON ANALYSIS

Version 1.0 860617

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REFERENCE MANUAL

1. Introduction

This document will provide a little more background information for the Robinson's analysis program.

This package contains all of the files needed to start running the analysis. It also contains all of the files necessary to modify the source code and compile and load a new version (assuming the presence of standard packages such as the editor, the fortran compiler and the loader). The intent is to supply the user with a working program so that he can start data analysis immediately and also to supply all of the source code so that further development and modifications can be performed.

2. History of the program

The source code for this analysis was obtained from Esso Research (Sarnia, Ont.) on a modem link. A copy was also obtained from the Research and Development Department of American Oil Co. (Whiting, Ind. where the program originated). These two copies were compared to verify the accuracy of the code which we obtained. The source code was loaded into the Nova 4 computer and the text editor, ED, was used to modify the program for use by the Super Incos data system. Although the function of the code has not been modified in any way there have been several major changes and a few minor changes made to enable use on the Nova 4. Once these changes were made a known data set was run through the analysis to verify operation of the program

3. Program Structure

The program now runs as six chained overlays on the Nova 4. Chaining is necessary because the code is too large to run as a single overlay. The main subroutines in the original version have become overlays in the current version. Most of the data previously passed to the various subroutines is now kept in a common area for all of the overlays.

The main program (ROBINS) provides the compatibility with the MSDS operating environment (command structure, error reporting, file access, etc.). It reads in the data and initiates the analysis. ROBINS calls a subroutine to deisotope the data (DEISO) and another routine to print the spectrum when required (PRSPEC). When this is done it chains to the next overlay, STERAN.

STERAN calls FUNCTION ST for base line sterane determinations. STERAN, in turn, chains to SATARM which calls subroutine BSLINE for base line calculations. SATARM chains to AROMAN which calls subroutines BALINE, SATINT, and RESOLVE. AROMAN chains to SATSAN which calls subroutines BLINE for base line calculations and SATMUL to do the matrix multiplication.

SATSAN chains back to AROMAN which chains back to SATSAN again for a second loop through these two routines. After the second pass through SATSAN the REPORT overlay is chained to produce the final results. When REPORT is done it chains back to ROBINS for new commands. The chain can be broken here by using any of the standard exit commands (E or ID or ^Z).

Below is a list of all 46 files included on the tape.

FCOPY.DS	to copy all files from one disk to another
ROBINS.MS	MSDS code for the main overlay
ROBINS.FR	source code for the main program
ROBINS.LD	loader file for the main overlay
ROBINS.PR	procedure to run analysis
STERAN.MS	MSDS code for STERAN overlay
SATARM.MS	MSDS code for SATARM overlay
REPORT.MS	MSDS code for REPORT overlay
AROMAN.MS	MSDS code for AROMAN overlay
SATSAN.MS	MSDS code for SATSAN overlay
TESTFILE.MI	a file of test data
TESTFILE.TI	time intensity original test data
CALIST.CT	calibration file to get above .MI file
EMR1.PR	procedure to run a number of analyses
EMR.PR	calls EMR1.PR
DEISO.FR	fortran source code for DEISO routine
EREX.FR	fortran source code for a system routine
BLINE.FR	fortran source code (subroutine)
STERAN.FR	fortran source code for STERAN routine
SATARM.FR	fortran source code for SATARM routine
REPORT.FR	fortran source code for REPORT routine

BALINE.FR	fortran source code (subroutine)
RESLOVE.FR	fortran source code (subroutine)
BSLINE.FR	fortran source code (subroutine)
SATINT.FR	fortran source code (subroutine)
AROMAN.FR	fortran source code for AROMAN routine
SATSAN.FR	fortran source code for SATSAN routine
FUNCTIONST.FR	fortran source code (subroutine)
PRSPEC.FR	fortran source code (subroutine)
ISHFT.SR	assembler source code for a system routine
OPLPT.SR	assembler source code for a system routine
GETIN.SR	assembler source code for a system routine
CMAIN.SR	assembler source code for a system routine
TPUSH.SR	assembler source code for a system routine
GCOPY.SR	assembler source code for a system routine
STERAN.LD	loader file for STERAN overlay
SATARM.LD	loader file for SATARM overlay
REPORT.LD	loader file for REPORT overlay
AROMAN.LD	loader file for AROMAN overlay
SATSAN.LD	loader file for SATSAN overlay
EXPLROBI.DS	help file for ROBINS
FRWRT.RB	binary code for a system file
FMRD.RB	binary code for a system file
FMCLS.RB	binary code for a system file
FMPOS.RB	binary code for a system file
FMOPN.RB	binary code for a system file

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       ROBINS.FR
C       Copyright (C) FINNIGAN MAT, 1984
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       History:
C
C       Date             Name             Description of Change
C
C
C       20 DEC 85        STEVE SIVERNS    IMPROVED DOCUMENTATION AND
C                                         ADDED LIMIT CHECK ON MASS
C       26 JULY 85                        DATED AS REVISION 1.0.
C
C       16 JLY 85        TOM WANG                 Created
C
C       Purpose:
C
C       This program does a mass spectral analysis of petroleum oils.
C
C       Run file is named:       ROBINS.MS
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       Associated files for this program:
C
C           SOURCE FILE     OBJECT FILE     RUN FILE
C
C           ROBINS.FR       ROBINS.RB       ROBINS.MS
C           DEISO.FR        DEISO.RB
C           PRSPEC.FR       PRSPEC.RB
C           STERAN.FR       STERAN.RB       STERAN.MS
C           FUNCTIONST.FR   FUNCTIONST.RB
C           SATARM.FR       SATARM.RB       SATARM.MS
C           BSLINE.FR       BSLINE.RB
C           AROMAN.FR       AROMAN.RB       AROMAN.MS
C           RESOLVE.FR      RESOLVE.RB
C           BALINE.FR       BALINE.RB
C           SATINT.FR       SATINT.RB
C           SATSAN.FR       SATSAN.RB       SATSAN.MS
C           BLINE.FR        BLINE.RB
C           SATMUL.FR       SATMUL.RB
C           REPORT.FR       REPORT.RB       REPORT.MS
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


        PARAMETER TTO=10, TTI=10, LPT=2, DSK=1  ;FORTRAN CHANNEL NO'S
        PARAMETER INPTLEN =6                    ;UP TO 6 INPUT NUMBERS
        PARAMETER OPENF=34K, RDWRD=30K, WRWRD=31K, TRUNF=32K, POSO=26K
        PARAMETER CLOSF=33K

        PARAMETER LMESS=12, NMESS=5             ;***1F
        PARAMETER PARAMSIZE=1                  ; NUMBER OF PARAMETERS IN FILE
        PARAMETER HIMASS=758                   ; MAXIMUM ACCEPTABLE MASS

        EQUIVALENCE
     1  (ITEMP14, ITEMP(14)), (DFILE16, DFILE(1,6)),
     1  (IN1, IN(1)), (IN2, IN(2)), (IN3, IN(3)),
     1  (FIN1, FIN(1)), (FIN2, FIN(2)), (FIN3, FIN(3)),
     1  (LASTPEAK, IDAT(45))
```

```
      COMMON /CERR/ MESS(LMESS, NMESS)
C     NOTE:  THE DECLARATIONS OF THE MAIN PROGRAM ARE HERE:
C
      INTEGER TITLE, INDAT(2)
C
C     END OF DECLARATIONS.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C  COMMON BLOCKS FOR CHAINING DATA TRANSFER
C

      COMMON /CDESC/
     1 METHODDESC(11),                    ;***4F
     1 MENUDESC(11),
     1 KEEPDESC(11)
      COMMON /CDATA/ IDATA
      COMMON /CKEEP/ AKEEP(PARAMSIZE) ;***6P

      COMMON /MAIN/ TITLE (2, 40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
     1 IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

      COMMON /COMPON/ SUMSS, PAR, CPAR, CCP, CCP2, CCP3, SUMAA,
     1 A6A, A10S, A20A,  A8A, A22A, A36A,  A10A, A24A, A38A,
     1 A12A, A16S, A26A,  A14A, A28A, A42A,  A16A, A30A, A44A,
     1 A18A, A22S, A32A,  BL1, BL2, BL3, BL4, AMON, DITRI, NPASS,
     1 SA1, SA2, SA3, SA4, A6, A7, A8, A9, A10, A11, C1, C2, C3,
     1 AA6, AA8, AA10, AA12, AA14, AA16, AA18,
     1 A12, A13, A14, A15, A16, A17, A18, A19


      COMMON /SASR/ S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI


      COMMON /CINPUT/ IDSW, INPUT, IFL, IBIT, IN(INPTLEN), FIN(INPTLEN)

      INTEGER DFSW, DFSW1, DFILE, SFILE

      COMMON /CMAIN/
     1 NPROG, DFSW, DFSW1, ITEMP(15),
     1 DFILE(12, 6), SFILE(11, 4),
     1 INSTD(3), IREFTABLE(11),
     1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISUB4,
     1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
     1 ISCN(45), IACQ(100), IDAT(45)

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      DATA METHODDESC  /"D<0>", 0, 1, "ROBINS", 2*0, "ME", 0/ ;***7F
      DATA MENUDESC    /"D<0>", 0, 1, "EXPLROBI", 0, 0, "DS", 0/
      DATA KEEPDESC    /"1<0>", 0, 1, "ROBINS", 2*0, "90", 0/

      DATA MESS(1, 1)  /"METHOD  XX"/  ;***8F
      DATA MESS(1, 2)  /"THE EXPLANATION FILE"/
      DATA MESS(1, 3)  /"KEEP FILE 0"/
      DATA MESS(1, 4)  /"DATA FILE"/

      LUO=TTO
      IFLAG1=0                            ;INITIALIZE FLAGS FOR RUNNING
      IFLAG2=0
      IFLAG3=0
      IFLAG4=0
      CALL GTINT(ICTR)
```

```
        IF(ICTR.EQ.0) GOTO 500
                                        ;THE USER TYPED CTRL-D OR CTRL-Z
        CALL CTOBF                      ;FLUSH TERMINAL OUTPUT BUFFER
        IF(ICTR.EQ.2000K) GOTO 100

        WRITE(TTO) "^D"
        GOTO 200

100     DFILE(1,5)=0                    ;CONTROL Z--STOP PROCEDURE
        WRITE(TTO) "^Z"

200     CALL RESET
        CALL TSAVE(DFILE16,$300,IE,IEE) ;REMEMBER LAST METHOD
300     CALL CTIBF                      ;CLEAR THE TERMINAL INPUT BUFFER

400     IDSW=.FALSE.
        GOTO 1000

CCC     "FIRST TIME THROUGH" CODE

500     IF(ITEMP14) GOTO 1000           ;RETURN FROM HARDCOPY OR OVERLAY
        INPUT=0
        IN1=0

C       "P" SUBCOMMAND
600     JCH=-1
        KEEPDESC(7)=(KEEPDESC(7).AND.177400K)+"<0>0"+IN1
        IERR=3
        MESS(6,IERR)="0"+ISHFT(IN1,8)
        IE=OPENF
        CALL FMOPR(KEEPDESC,JCH,$700,IEE)
        IE=RDWRD
        CALL FMRD(AKEEP,JCH,PARAMSIZE,$700,IEE)
        CALL FMCLS(JCH,$900,IEE)
        GOTO 900

700     IF (INPUT) GOTO 2100    ;DON'T REPORT ERROR ON INITIAL "P"

CCC     "I" SUBCOMMAND

800     AKEEP(1)=1.0                    ;DEFAULT AINF TO 1.0

CCC     COMMAND PROCESSOR

900     IDSW=.TRUE.                     ;PREPARE TO DISPLAY IN CASE
                                        ;THERES NO INPUT
1000    CALL STINT(6000K)               ;ALLOW ^D AND ^Z
        CALL IGETIN(INPUT,IFL,IBIT,INPTLEN,IN,FIN,$200,$1100)
        GOTO 1300                       ;INPUT WAITING AT TERMINAL
                                        ;OR IN METHOD

1100    I=DFILE16                       ;IF EOF AT END OF METHOD,
        IERR=1                          ;TRY TO POP THE METHOD
        MESS(5,IERR)=ISHFT(DFILE(7,6),8)+ISHFT(DFILE(8,6),-8)
        CALL TPOP(DFILE16,$2100,IE,IEE)

        IF(I) GOTO 1000                 ;WE POPPED TO ANOTHER METHOD
        IF(IDSW) GOTO 3000              ;NO INPUT, DISPLAY IF REQUESTED

        WRITE(TTO,1200)
1200    FORMAT(1X,"ROBINS: "Z)
        CALL IGET1(INPUT,IFL,IBIT,INPTLEN,IN,FIN,$200,$1100)
```

```
1300    DO 1400 II=1, INPTLEN     ;INTERPRET !'S AS MSDS VARIABLES (10-19)
        IF(IFL. NE. "! ")GOTO 1400          ;DONT BOTHER IF WE HAVENT GOT !

        N=IABS(IN(II))            ;GOT A !
        IF(N. LT. 10. OR. N. GT. 19) GOTO 1400  ;IGNORE !'S IF NOT 10-19

        MINUS=1-2*IABS(IN(II). LT. 0)
        IN(II)=MINUS*SFILE(N-8, 4)
        FIN(II)=IN(II)

1400    CONTINUE

        GOTO 3400                                     ;DISPATCH TABLE

CCC     "?" SUBCOMMAND

1500    KCHAN=TTO
        WRITE(TTO, 3100) ;CLEAR SCREEN
        GOTO 1700

CCC     "Q" SUBCOMMAND

1600    KCHAN=LPT
        IE=OPENF
        CALL OPLPT(LPT, $2100)

1700    IE=OPENF                          ;COPY MENU TO SCREEN OR PRINTER
        IERR=2
        ICH=-1
        CALL FMOPR(MENUDESC, ICH, $2100, IEE)
        IE=0
        CALL GCOPY(ICH, KCHAN, $2100, IE, IEE)
        IE=CLOSF
        CALL FMCLS(ICH, $2100, IEE)
        CALL CLOSE(DSK, IEE)
        IF(KCHAN. NE. LPT) GOTO 400

        WRITE(LPT, 3100, ERR=1800)      ;ALWAYS DO ONE FORM FEED ON PRINTER
        IF(IFL. EQ. "^ ") WRITE (LPT, 3100, ERR=1800) ;EXTRA FORM FEED
1800    CALL CLOSE(LPT, IE)
        GOTO 400


CCC     METHOD HANDLER


1900    IF(INPUT. EQ.  0) GOTO 2000                   ;RESTART CURRENT METHOD

        IF((INPUT. AND. 377K). EQ. 40K) INPUT=INPUT-40K ;START NEW METHOD
        METHODDESC(7)=(METHODDESC(7). AND. 177400K)+ISHFT(INPUT, -8)
        METHODDESC(8)=ISHFT(INPUT, 8)
        IERR=1
        MESS(5, IERR)=INPUT
        CALL TPUSH(DFILE16, $2100, IE, IEE, METHODDESC)
        GOTO 1000                                     ;(COMMAND PROCESSOR)

2000    CALL TSOUR(I)                     ;GET THE IDOS CHANNEL
        IF(I. LT. 1) GOTO 1000            ;NO METHOD RUNNING-CAN'T RESTART

        IE=POSO                           ;"REWIND" METHOD
        IERR=1
        MESS(5, IERR)=ISHFT(METHODDESC(7), 8)+ISHFT(METHODDESC(8), -8)
        CALL FMPOS(0, 24, I, $2100, IEE)
        GOTO 1000
```

```
CCC     ERROR HANDLER


2100    CALL EREX(IEE, IE, MESS(1, IERR), LMESS)     ;VARIOUS ERRORS
        GOTO 200

CCC     "E" SUBCOMMAND -- EXIT TO MSDS EXEC

2200    IBUF=0
        IEXIT=1
        GOTO 2500

CCC     "ID" SUBCOMMAND -- EXIT TO IDOS

2300    IEXIT=-1
        GOTO 2500

CCC     "K" SUBCOMMAND -- KEEP PARAMETERS IN DISK FILE

2400    IEXIT=0
2500    JCH=-1
        IF (IN1. LT. 0. OR. IN1. GT. 9) GOTO 1500
        KEEPDESC(7)=(KEEPDESC(7). AND. 177400K)+"<0>0"+IN1
        IERR=3
        MESS(6, IERR)="0"+ISHFT(IN1, 8)
        IE=OPENF
        CALL FMOPN(KEEPDESC, JCH, $2700, IEE)
        IE=WRWRD
        CALL FMWRT(AKEEP, JCH, PARAMSIZE, $2700, IEE)
        GOTO 2800

2700    IF (IEXIT. EQ. 0) GOTO 2100
2800    CALL FMCLT(JCH, $2900, IEE)

2900    IF (IEXIT. EQ. 0) GOTO 1000
        IF (IEXIT. LT. 0) CALL EXIT
        CALL LOADIT("EXEC")



CCC     DISPLAY


3000    KCHAN=TTO
        LUO=TTO
        WRITE(TTO, 3100)
3100    FORMAT(" "Z)                          ;CLEAR-SCREEN FORMAT
        GOTO 3300


CCC     HARDCOPY


3200    KCHAN=LPT
        LUO=LPT
        CALL OPLPT(LPT, $2100)
3300    IDSW=. FALSE.



CCC     DISPLAY AND HARDCOPY CODE INSERTED HERE ;***10D
```

```
        GOTO 1000

CCC     COMMAND PROCESSOR

3400    IF (INPUT.EQ."ID") GOTO 2300        ;***11I
        IF (IFL.EQ."@ ") GOTO 1900          ;READ IN A METHOD
        IF (IFL.EQ."? ") GOTO 1500          ;DISPLAY EXPLANATION PAGE
                                            ;***12I
        IF(INPUT.EQ.0) GOTO 1000            ;GO BACK FOR MORE INPUT

        ICC=INPUT/256-"<0>@"
        IF(ICC.LT.1.OR.ICC.GT.26) GOTO 1500
        GOTO(
     1  5015,    ;A                         DO ANALYSIS
     1  1500,    ;B
     1  1500,    ;C
     1  3000,    ;D                         DISPLAY VALUES
     1  2200,    ;E                         EXIT TO MSDS
     1  1500,    ;F
     1  5000,    ;G                         READ AND DO ANALYSIS
     1  3200,    ;H                         HARDCOPY DISPLAY
     1  800,     ;I                         INITIALIZE PARAMETERS
     1  1500,    ;J
     1  2400,    ;K                         KEEP PARAMETERS IN A DISK FILE
     1  5010,    ;L                         LIST FULL SPECTRUM
     1  1500,    ;M
     1  1500,    ;N
     1  1500,    ;O
     1  600,     ;P                         READ PARAMETERS FROM KEEP FILE
     1  1600,    ;Q                         HARDCOPY EXPLANATION FILE
     1  5005,    ;R                         READ IN THE SPECTRUM
     1  8000,    ;S                         SET PARAMETERS (AINF ONLY)
     1  7000,    ;T                         PRINT INTERMEDIATES (DEBUG)
     1  1500,    ;U
     1  1500,    ;V
     1  1500,    ;W
     1  1500,    ;X
     1  1500,    ;Y
     1  1500)ICC ;Z

C*************************************************************************
C
C         HERE LIES ALL OF THE PROCESS SPECIFIC CODE
C
C*************************************************************************
C
C
5000    IFLAG2=1      ; READ AND THEN DO ANALYSIS
5005    ICH= -1       ; TAKE ANY CHANNEL
        IERR=4        ; WE ARE USING THE 4TH FILE (DATA FILE)
        IE=OPENF      ; CODE FOR ERROR REPORT

C   OPEN THE MAIN DATA FILE (DESC IN SFILE(N,1) )

        SFILE(10,1)="MI"       ; FORCE .MI TYPE FILE
        CALL FMOPR (SFILE(1,1),ICH,$2100,IEE)

        DO 20 J=1,2
        DO 20 I=1,40
   20   TITLE(J,I)=0     ; CLEAR THE TITLE LINES FOR NEW DATA

        MASS = 0
        DO 30 I=1,HIMASS
        H(I)=0.0     ; THIS LOOP CLEARS THE ARRAYS FOR THE PEAK
   30   HDI(I)=0.0  ; HEIGHTS FOR STANDARD AND DEISOTOPED SAMPLES
```

```
          IE=RDWRD      ; SET UP FOR READ
          CALL FMRD(ISCN, ICH, 190, $2100, IEE)      ; READ HEADER FROM FILE

C    LAST 3 ARRAYS OF CMAIN ARE INITIALIZED.  LASTPEAK IS IN ONE
C     OF THESE (SEE EQUIVALENCES AT TOP).


          DO 50 I=1, LASTPEAK       ; MAKE SURE ALL PEAKS ARE READ
          IE=POSO
          CALL FMPOS(0, 380+I*4, ICH, $2100, IEE)    ; POSITION FILE POINTER
          IE=RDWRD
          CALL FMRD(INDAT, ICH, 2, $2100, IEE)       ; NOW READ IN PEAK DATA.

          IF(INDAT(1). LT. 0) GO TO 70      ; IF AT END THEN QUIT.
          MASS=MASS+INDAT(2)                ; NEW MASS
          IF(MASS . GT.  HIMASS) GOTO 70       ; TOO BIG FOR ARRAYS
          IEXP=INDAT(1)/512
          IR=INDAT(1)-IEXP*512              ; CONVERT DATA FROM CORE
          H(MASS)=INDAT(1)                  ; TO FLOATING POINT FORMAT
          IF(IEXP. GT. 0) H(MASS)=FLOAT(IR+512)*2**(IEXP-1)
    50    CONTINUE

    70    IE=CLOSF
          CALL FMCLS(ICH, $2100, IEE)       ; CLOSE WHAT YOU OPENED.

          IFLAG1=1          ; SET DATA AVAILABLE FLAG
          H(28)=0           ; REMOVE NITROGEN
          H(32)=0           ; REMOVE OXYGEN
          SUMH=0. 0

          DO 80 I=24, HIMASS
    80    SUMH=SUMH+H(I)        ; ADD UP SUM OF PEAKS AFTER CLEARING VARIABLE.


C    GET TITLE INFORMATION FROM HEADER INFO

          DO 85 I=1, 6                  ; GET FILE NAME FROM HEADER
    85    TITLE(1, I)=ISCN(I+3)

          TITLE(1, 7)=". "
          TITLE(1, 8)=ISCN(10)          ; GET FILE EXTENSION
          TITLE(1, 9)="  "              ; LEAVE SPACES

          DO 90 I=1, 4
    90    TITLE(1, 11+I)=IACQ(I)    ; GET FILE CREATION DATE

          DO 95 I=1, 16
    95    TITLE(2, I)=IACQ(9+I)       ; GET TEXT

          CALL DEISO                     ; DEISOTOPE THE PEAKS

          IF(IFLAG2. NE. 0) GO TO 5015    ; DO ANALYSIS
          GO TO 1000                      ; ELSE GO BACK FOR ANOTHER COMMAND

 5010     IF (IFLAG1 . EQ.  0) GO TO 1000  ;DATA WAS NOT READ IN

          CALL PRSPEC ;  OUTPUT LIST OF FULL SPECTRUM VALUES
          GO TO 1000          ; THEN GO BACK FOR ANOTHER COMMAND.

 5015     IF (IFLAG1 . EQ.  0) GO TO 1000  ;DATA WAS NOT READ IN
          AVMLWT=FIN1                     ;GET MOL WT FROM MSDS INPUT DATA

          CALL LOADIT("STERAN")     ; RUN ROBINSON'S ANALYSIS
C
C    SET FLAG FOR DEBUG PRINTING
```

```
C
 7000   IFLAG4=1
        GO TO 1000
C
C   SET NEW PARAMETERS
C
 8000   WRITE(TTO,8010)AKEEP(1)
 8010   FORMAT(" ENTER A VALUE FOR AINF (",F10.4,"): "Z)
        READ(TTO,8020) AKEEP(1)
 8020   FORMAT(F12.3)
        GO TO 1000

        END
```

```
       PARAMETER HIMASS = 758

      SUBROUTINE DEISO

C
C     REVISION 1.0 AS OF 260785
C     REVISION 1.1 AS OF 851220 SS ADDED DOCUMENTATION
C


C
C   THIS SUBROUTINE COMPUTES MONOISOTOPIC PEAKS ASSUMING ALL IONS ARE
C     COMPOSED OF Z NUMBERS +2 TO -11.
C
C   THE METHOD IS REFERENCED IN: ROBINSON & COOK, ANALYTICAL CHEM.
C     VOL 41 #12, OCT. 1969, P 1549.
C

      INTEGER TITLE  ;850710 TW TITLE CHANGE.

      COMMON /MAIN/ TITLE(2,40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
     1IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

      COMMON /SASR/ NCARB(HIMASS), NHYD(HIMASS), SR(HIMASS),
     1 AVMLWT, STIV, STV, STVI

C
C    SASR FIRST TWO ARRAYS ARE USED TEMPORARILY HERE TO REDUCE STACK
C                850724 SS
C
      DO 1 I=11,758              ; ZERO ALL ARRAYS
      HDI(I) = 0.0
      NCARB(I) = 0
    1 NHYD(I) = 0

      DO 1011 K = 12,758
      NCARB(K) = (K + 11)/14     ; NUMBER OF CARBONS AT THIS MASS
      NHYD(K) = K - 12*NCARB(K)  ; NUMBER OF HYDROGENS AT THIS MASS
      IF(NHYD(K).LT.0) NHYD(K) = 0  ; CAN'T BE NEGATIVE
 1011 CONTINUE

C    THESE EQUATIONS DO THE DEISOTOPING

      DO 1015 K = 14,758
      HDI(K) = H(K)-HDI(K-1)*(.010811*FLOAT(NCARB(K-1))+.00015*FLOAT
     1(NHYD(K-1)))
      HDI(K) = HDI(K)+HDI(K-2)*(.00005844*FLOAT(NCARB(K-2)*(1-NCARB(K-2)
     1))+.1125E-7*FLOAT(NHYD(K-2)*(1-NHYD(K-2)))-.162165E-5*FLOAT(NCARB(
     2K-2)*NHYD(K-2)))
      IF(HDI(K).LT.0.0)HDI(K) = 0.0
 1015 CONTINUE

      SUMHDI = 0.0
      DO 1016 K = 14,758
 1016 SUMHDI = SUMHDI + HDI(K)   ; SUM OF DEISOTOPED PEAKS

      RETURN
      END
```

```
         PARAMETER HIMASS=758      ; HIGHEST MASS ALLOWED

        SUBROUTINE PRSPEC


C
C     REVISION 1.0 AS OF 260785
C
C     REVISION 1.1 851220 SS   CHANGED NAME FROM MATRIX TO PRSPEC
C                               AND IMPROVED DOCUMENTATION
C
C     CALLED BY "ROBINS"
C     REQUIRES H(I), HDI(I), SUMH, TITLE


C
C   THIS ROUTINE PRINTS THE MASS SPECTRUM IN 7 COLUMNS
C
        INTEGER TITLE  ;850710 TW TITLE CHANGE..

        COMMON /MAIN/ TITLE(2,40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
       1IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

        DIMENSION MASS(7), PEAK(7), PK(7)

C   PK(I) REPRESENTS MONOISOTOPIC PEAK

        WRITE(LUO,2)((TITLE(J,I),I=1,40),J=1,2), SUMH, SUMHDI
        WRITE (LUO,1)
      1 FORMAT(' ',15X,53HMASS SPECTRUM:   TOP-POLYISOTOPIC, BOTTOM-MONOISO
       1TOPIC/////)
      2 FORMAT(//,2(1H ,40A2/),1H /10X,44HSUM OF POLY AND MONO PEAKS FOR TH
       1IS TABLE:   ,2F10.0/)

        ENDSUM = 0.0
        DO 30 I=12,758          ; FIND THE HIGHEST MASS PRESENT
        ENDSUM = ENDSUM + H(I)
        IF(ENDSUM.GE.SUMH)GO TO 31
     30 CONTINUE

     31 MAXMAS = I                ; HIGHEST MASS PRESENT
        DO 10 I=17,MAXMAS,7       ; DO 7 AT A TIME
        II = I+6
        L = 0

        DO 20 J=I,II
        L = L+1
        MASS(L) = J               ; THE MASS
        PEAK(L) = H(J)            ; THE PEAK HEIGHT
        PK(L) = HDI(J)            ; THE DEISOTOPED PEAK HEIGHT
     20 CONTINUE

        WRITE(LUO,51)(MASS(M),M=1,7)
        WRITE(LUO,52)(PEAK(M),M=1,7)
        WRITE(LUO,53)(PK(M),M=1,7)
     51 FORMAT(1H ,7(I8,2X))
     52 FORMAT(1H ,7(F10.1))
     53 FORMAT(1H ,1X,7(F10.2)//)
     10 CONTINUE

        RETURN
        END
```

```
C        SUBROUTINE STERAN

C           OVERLAY STERAN        CHAINED FROM ROBINS
C                                 CHAINS TO SATARM

C
C     REVISION 1.0 AS OF 260785
C


C
C    THIS ROUTINE ESTIMATES PEAK SUMS DUE TO STERANES(STIV), PENTACYCLIC
C      TRITERPANES(STV), AND HEXACYCLIC TRITERPANES(STVI).

       PARAMETER HIMASS=758
       PARAMETER PARAMSIZE=1
       PARAMETER INPTLEN=6
C
       INTEGER TITLE  ;850710 TW TITLE CHANGE.

       COMMON /CDESC/        ;INFILE(11),
      1 METHODDESC(11),
      1 MENUDESC(11),
      1 KEEPDESC(11)

       COMMON /CDATA/ IDATA
       COMMON /CKEEP/ AKEEP(PARAMSIZE)

       COMMON /MAIN/ TITLE(2,40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
      1IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

       COMMON /COMPON/ SUMSS, PAR, CPAR, CCP, CCP2, CCP3, SUMAA,
      1 A6A, A10S, A20A,  A8A, A22A, A36A,  A10A, A24A, A38A,
      1 A12A, A16S, A26A,  A14A, A28A, A42A,  A16A, A30A, A44A,
      1 A18A, A22S, A32A,  BL1, BL2, BL3, BL4, AMON, DITRI, NPASS,
      1 SA1, SA2, SA3, SA4, A6, A7, A8, A9, A10, A11, C1, C2, C3,
      1 AA6, AA8, AA10, AA12, AA14, AA16, AA18,
      1 A12, A13, A14, A15, A16, A17, A18, A19


       COMMON/SASR/S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI

       COMMON /CINPUT/ IDSW, INPUT, IFL, IBIT, IN(INPTLEN), FIN(INPTLEN)

       INTEGER DFSW, DFSW1, DFILE, SFILE

       COMMON /CMAIN/
      1 NPROG, DFSW, DFSW1, ITEMP(15),
      1 DFILE(12,6), SFILE(11,4),
      1 INSTD(3), IREFTABLE(11),
      1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISUB4,
      1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
      1 ISCN(45), IACQ(100), IDAT(45)

       DIMENSION PEAK(9)

       STIV = 0.0
       STV = 0.0
       STVI = 0.0
       IF(H(386).EQ.0.0)GO TO 39

       J = 0

       DO 10 I=330,442,14
       J = J+1
```

```
10 PEAK(J) = H(I)

   STA = ST(PEAK)
   IF(STA.EQ.0.0)GO TO 18
   C218 = (H(204) - (H(204)-H(246))/3.0)
   IF(H(218).GT.C218)STIV=STIV+H(218)-C218
   IF(H(218).LT.C218)C218=H(218)
   C232 = (C218 + H(246))/2.0
   IF(H(232).GT.C232)STIV=STIV+H(232)-C232
   C260 = (H(246)+H(274))/2.0
   IF(H(260).GT.C260)STIV=STIV+H(260)-C260
   STIV = STIV + STA
   C217 = (HDI(203) - (HDI(203)-HDI(245))/3.0)
   IF(HDI(217).GT.C217)STIV=STIV+HDI(217)-C217
   IF(HDI(217).LT.C217)C217=HDI(217)
   C231 = (C217 + HDI(245))/2.0
   IF(HDI(231).GT.C231)STIV=STIV+HDI(231)-C231
   C259 = (HDI(245) + HDI(273))/2.0
   IF(HDI(259).GT.C259)STIV=STIV+HDI(259)-C259
   J = 0

   DO 11 I=329,441,14
   J = J + 1
11 PEAK(J) = HDI(I)

   STIV = STIV + ST(PEAK)
   GO TO 19

18 STIV = 0.0

19 J = 0

   DO 20 I=328,440,14
   J = J + 1
20 PEAK(J) = H(I)

   STA = ST(PEAK)
   IF(STA.EQ.0.0)GO TO 28
   C258 = (H(244)+H(272))/2.0
   IF(H(258).GT.C258)STV=STV+H(258)-C258
   C257 = (HDI(243)+HDI(271))/2.0
   IF(HDI(257).GT.C257)STV=STV+HDI(257)-C257
   STV = STV + STA
   J = 0

   DO 21 I=327,439,14
   J = J + 1
21 PEAK(J) = HDI(I)

   STV = STV + ST(PEAK)
   GO TO 29

28 STV = 0.0

29 J = 0
   DO 30 I=326,438,14
   J = J + 1
30 PEAK(J) = H(I)

   STA = ST(PEAK)
   IF(STA.EQ.0.0)GO TO 38
   C256 = (H(242) + H(270))/2.0
   IF(H(256).GT.C256)STVI=STVI+H(256)-C256
   C255 = (HDI(241) + HDI(269))/2.0
   IF(HDI(255).GT.C255)STVI=STVI+HDI(255)-C255
   STVI = STVI + STA
   J = 0

   DO 31 I=325,437,14
   J = J + 1
31 PEAK(J) = HDI(I)

   STVI = STVI + ST(PEAK)
   GO TO 39

38 STVI = 0.0

39 CALL LOADIT("SATARM")
   END
```

```
      FUNCTION ST(PEAK)
C
C    REVISION 1.0 AS OF 260785
C

      DIMENSION PEAK(9),PK(9)
      J = 0
      K = 1
      DO 1 I=1,9
      IF(PEAK(I).EQ.0)GO TO 7
    1 CONTINUE
      L = 9
      GO TO 4
    7 L = I - 1
      IF(L.LT.5)GO TO 90
      GO TO 4
    2 K = K + 1
      J = 1
      GO TO 4
    3 L = L - 1
      J = 0
    4 KK = K + 1
      LL = L - 1
      DELTA =(PEAK(K)-PEAK(L))/FLOAT(L-K)
      N = 0
      DO 10 I=K,L
      PK(I) = PEAK(K) - FLOAT(N)*DELTA
   10 N = N + 1
      IF(LL.EQ.KK)GO TO 70
      IF(PK(KK).LT.PEAK(KK))GO TO 20
      IF(PK(LL).LT.PEAK(LL))GO TO 30
      IF(J)2,2,3
   20 IF(PK(LL).LT.PEAK(LL))GO TO 70
      L = L - 1
      GO TO 4
   30 IF(PK(KK).LT.PEAK(KK))GO TO 70
      K = K + 1
      GO TO 4
   70 ST = 0.0
      DO 71 I=KK,LL
      STB = PEAK(I) - PK(I)
      IF(STB.LT.0.0)STB=0.0
   71 ST = ST + STB
      GO TO 99
   90 ST = 0.0
   99 RETURN
      END
```

```
C       SUBROUTINE SATARM
C         OVERLAY SATARM          CHAINED BY STERAN
C                                 CHAINS TO AROMAN
C
C     REVISION 1.0 AS OF 260785
C               1.1      860210    ; ADDED HIMASS AND CLEANED UP
C
C
C  CALCULATES A SATURATES SPECTRUM AND AN AROMATICS SPECTRUM
C   IF IFLAG4 = 1, S(M) AND A(M) ARE PRINTED.
C
        PARAMETER INPTLEN =6
        PARAMETER HIMASS=758
        PARAMETER PARAMSIZE=1

        COMMON /CDESC/       ;INFILE(11),
       1 METHODDESC(11),
       1 MENUDESC(11),
       1 KEEPDESC(11)

        COMMON /CDATA/IDATA
        COMMON /CKEEP/ AKEEP(PARAMSIZE)

        INTEGER TITLE  ;850710 TW TITLE CHANGE.

        COMMON /MAIN/ TITLE(2,40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
       1IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

        COMMON /COMPON/ SUMSS, PAR, CPAR, CCP, CCP2, CCP3, SUMAA,
       1 A6A, A10S, A20A,  A8A, A22A, A36A,  A10A, A24A, A38A,
       1 A12A, A16S, A26A,  A14A, A28A, A42A,  A16A, A30A, A44A,
       1 A18A, A22S, A32A,  BL1, BL2, BL3, BL4, AMON, DITRI, NPASS,
       1 SA1, SA2, SA3, SA4, A6, A7, A8, A9, A10, A11, C1, C2, C3,
       1 AA6, AA8, AA10, AA12, AA14, AA16, AA18,
       1 A12, A13, A14, A15, A16, A17, A18, A19


        COMMON/SASR/S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI

        COMMON /CINPUT/ IDSW, INPUT, IFL, IBIT, IN(INPTLEN), FIN(INPTLEN)

        INTEGER DFSW, DFSW1, DFILE, SFILE

        COMMON /CMAIN/
       1 NPROG, DFSW, DFSW1, ITEMP(15),
       1 DFILE(12,6), SFILE(11,4),
       1 INSTD(3), IREFTABLE(11),
       1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISUB4,
       1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
       1 ISCN(45), IACQ(100), IDAT(45)

        EQUIVALENCE
       1 (S93, S(93)), (S107, S(107)), (S121, S(121)),
       1 (S135, S(135)), (S149, S(149)), (S94, S(94)),
       1 (S108, S(108)), (S122, S(122)), (S136, S(136)),
       1 (S81, S(81)), (S95, S(95)), (S82, S(82)),
       1 (S96, S(96)), (S110, S(110)), (S124, S(124)),
       1 (S55, S(55)), (S69, S(69)), (S83, S(83)),
       1 (S97, S(97)), (S111, S(111)), (S125, S(125)),
       1 (S70, S(70)), (S84, S(84)), (S43, S(43)),
       1 (S57, S(57)), (S71, S(71)), (S85, S(85)),
     1 (S99, S(99)),
     1 (HDI79, HDI(79)), (HDI93, HDI(93)), (HDI107, HDI(107)),
     1 (HDI121, HDI(121)), (HDI135, HDI(135)), (HDI149, HDI(149)),
     1 (HDI95, HDI(95)), (HDI125, HDI(125)), (HDI85, HDI(85)),
     1 (HDI99, HDI(99)),
     1 (H80, H(80)), (H94, H(94)), (H108, H(108)),
     1 (H122, H(122)), (H136, H(136)), (H67, H(67)),
     1 (H81, H(81)), (H95, H(95)), (H68, H(68)),
     1 (H82, H(82)), (H96, H(96)), (H110, H(110)),
     1 (H124, H(124)), (H55, H(55)), (H69, H(69)),
     1 (H83, H(83)), (H97, H(97)), (H111, H(111)),
     1 (H125, H(125)), (H56, H(56)), (H70, H(70)),
     1 (H84, H(84)), (H43, H(43)), (H57, H(57)),
     1 (H71, H(71)), (H85, H(85))

      DO 1 I=12, HIMASS
      S(I) = 0. 0
    1 A(I) = 0. 0
C
C   MAKE PATTERN FIT FOR MASSES 93 THRU 149
C
      S93 = . 86*HDI79
      IF(HDI93. LT. S93)S93=HDI93
      S107 = . 64*HDI79
      IF(HDI107. LT. S107)S107=HDI107
      S121 = . 53*HDI79
      IF(HDI121. LT. S121)S121=HDI121
      S135 = . 52*HDI79
      IF(HDI135. LT. S135)S135=HDI135
      P = . 79*S93
      IF(P. LT. S107)S107=P
      P = . 75*S93
      IF(P. LT. S121)S121=P
      P = . 73*S93
      IF(P. LT. S135)S135=P
      P = . 9*S107
      IF(P. LT. S121)S121=P
      IF(P. LT. S135)S135=P
      IF(S121. LT. S135)S135=S121
      S149 = . 95*S135
      IF(HDI149. LT. S149)S149=HDI149
C
C   MAKE PATTERN FIT FOR MASSES 94 THRU 136
C
      S94 = H80
      IF(H94. LT. S94)S94=H94
      S108 = . 9*H80
      IF(H108. LT. S108)S108=H108
      S122 = . 75*H80
      IF(H122. LT. S122)S122=H122
      S136 = . 63*H80
      IF(H136. LT. S136)S136=H136
      P = . 81*S94
      IF(P. LT. S108)S108=P
      P = . 67*S94
      IF(P. LT. S122)S122=P
      P = . 61*S94
      IF(P. LT. S136)S136=P
      P = . 83*S108
      IF(P. LT. S122)S122=P
      P = . 8*S108
      IF(P. LT. S136)S136=P
      P = . 96*S122
      IF(P. LT. S136)S136=P
C
C   MAKE PATTERN FIT FOR MASSES 81 AND 95
```

```
      S81 = 1. 25*H67
      IF(H81. LT. S81)S81=H81
      S95 = 1. 17*H67
      IF(H95. LT. S95)S95=H95
      P = . 94*S81
      IF(P. LT. S95)S95=P
      S95 = HDI95-(H95-S95)
C
C  MAKE PATTERN FIT FOR MASSES 82 THRU 124
C
      S82 = 1. 4*H68
      IF(H82. LT. S82)S82=H82
      S96 = 1. 1*H68
      IF(H96. LT. S96)S96=H96
      S110 = . 66*H68
      IF(H110. LT. S110)S110=H110
      S124 = . 43*H68
      IF(H124. LT. S124)S124=H124
      P = . 83*S82
      IF(P. LT. S96)S96=P
      P = . 53*S82
      IF(P. LT. S110)S110=P
      P = . 35*S82
      IF(P. LT. S124)S124=P
      P = . 64*S96
      IF(P. LT. S110)S110=P
      P = . 42*S96
      IF(P. LT. S124)S124=P
      P = . 66*S110
      IF(P. LT. S124)S124=P
C
C  MAKE PATTERN FIT FOR MASSES 55 THRU 125
C
      S55 = H55
      S69 = . 69*H55
      IF(H69. LT. S69)S69=H69
      S83 = . 51*H55
      IF(H83. LT. S83)S83=H83
      S97 = . 43*H55
      IF(H97. LT. S97)S97=H97
      S111 = . 24*H55
      IF(H111. LT. S111)S111=H111
      S125 = . 13*H55
      IF(H125. LT. S125)S125=H125
      P = . 79*S69
      IF(P. LT. S83)S83=P
      P = . 68*S69
      IF(P. LT. S97)S97=P
      P = . 36*S69
      IF(P. LT. S111)S111=P
      P = . 19*S69
      IF(P. LT. S125)S125=P
      P = . 87*S83
      IF(P. LT. S97)S97=P
      P = . 5*S83
      IF(P. LT. S111)S111=P
      P = . 28*S83
      IF(P. LT. S125)S125=P
      P = . 58*S97
      IF(P. LT. S111)S111=P
      P = . 33*S97
      IF(P. LT. S125)S125=P
      P = . 54*S111
      IF(P. LT. S125)S125=P
      S125 = HDI125-(H125-S125)
```

```
C
C   MAKE PATTERN FIT FOR MASSES 70 AND 84
C
      S70 = . 69*H56
      IF(H70. LT. S70)S70=H70
      S84 = . 38*H56
      IF(H84. LT. S84)S84=H84
      P = . 57*S70
      IF(P. LT. S84)S84=P
C
C   MAKE PATTERN FIT FOR MASSES 43 THRU 99
C
      S43 = H43
      S57 = . 9*H43
      IF(H57. LT. S57)S57=H57
      S71 = . 44*H43
      IF(H71. LT. S71)S71=H71
      S85 = . 27*H43
      IF(H85. LT. S85)S85=H85
      P = . 52*S57
      IF(P. LT. S71)S71=P
      P = . 32*S57
      IF(P. LT. S85)S85=P
      P = . 63*S71
      IF(P. LT. S85)S85=P
      S99 = . 206*(HDI85-(H85-S85))
      IF(HDI99. LT. S99)S99=HDI99
C
C   FILL REMAINING VALUES IN "S" ARRAY USING BASE LINE METHOD OF OBTAININ
C     SATURATES - AROMATIC SPLIT.
C
      CALL BSLINE  (149, 0. 514, 45. 04, HDI)
      CALL BSLINE  (136, 1. 16, 54. 07, H)
      CALL BSLINE  (95, 0. 211, 110. 8, HDI)
      CALL BSLINE  (124, 0. 85, 65. 04, H)
      CALL BSLINE  (125, 0. 15, 64. 00, HDI)
      CALL BSLINE  (84, 0. 7786, 141. 71, H)
      CALL BSLINE  (99, 1. 0, 102. 03, HDI)
C
C   PRELIMINARY VALUES HAVE BEEN ENTERED IN THE "S" ARRAY.  DEVIATIONS
C     FROM LINEARITY ARE NEXT ACCOUNTED FOR USING PEAK-BY-PEAK CORRETIONS
C
      S(163) = S(163)*2. 02
      S(177) = S(177)*1. 9
      S(191) = S(191)*2. 02
      S(205) = S(205)*1. 53
      S(219) = S(219)*1. 51
      S(233) = S(233)*1. 37
      S(247) = S(247)*1. 36
      S(261) = S(261)*1. 31
      S(275) = S(275)*1. 22
      S(289) = S(289)*1. 18
      S(303) = S(303)*1. 1
C
      S(150) = S(150)*. 954
      S(164) = S(164)*. 875
      S(178) = S(178)*. 854
      S(192) = S(192)*. 865
      S(206) = S(206)*. 87
      S(220) = S(220)*. 9
      S(234) = S(234)*. 95
C
      S(109) = S(109)*3. 85
      S(123) = S(123)*3. 11
      S(137) = S(137)*2. 54
      S(151) = S(151)*2. 29
      S(165) = S(165)*2.08
      S(179) = S(179)*1.9
      S(193) = S(193)*1.9
      S(207) = S(207)*1.57
      S(221) = S(221)*1.42
      S(235) = S(235)*1.4
      S(249) = S(249)*1.37
      S(263) = S(263)*1.37
      S(277) = S(277)*1.2
      S(291) = S(291)*1.1
C
      S(138) = S(138)*.932
      S(152) = S(152)*.862
      S(166) = S(166)*.854
      S(180) = S(180)*.9
      S(194) = S(194)*.94
      S(208) = S(208)*.96
C
      S(139) = S(139)*3.2
      S(153) = S(153)*2.37
      S(167) = S(167)*2.13
      S(181) = S(181)*2.0
      S(195) = S(195)*2.0
      S(209) = S(209)*1.57
      S(223) = S(223)*1.42
      S(237) = S(237)*1.42
      S(251) = S(251)*1.33
      S(265) = S(265)*1.25
      S(279) = S(279)*1.14
      S(293) = S(293)*1.07
C
      S(98) = S(98)*1.2
      S(112) = S(112)*1.23
      S(126) = S(126)*1.17
      S(140) = S(140)*.93
      S(154) = S(154)*.85
      S(168) = S(168)*.9
C
      S(127) = S(127)*.946
      S(141) = S(141)*.896
      S(155) = S(155)*.889
      S(169) = S(169)*.944
C
C  ALL DATA IN THE "S" ARRAY HAVE BEEN CORRECTED FOR LINEARITY DEVIATION
C    IT IS NECESSARY THAT NO VALUE IN THE "S" ARRAY EXCEED THE VALUE AT
C    THE SAME MASS IN THE "H" ARRAY FOR EVEN MASSES AND THE "HDI" ARRAY
C    FOR ODD MASSES.
C
      DO 2 I=163,HIMASS,14
      IF(HDI(I).LT.S(I))S(I)=HDI(I)
    2 CONTINUE
      DO 3 I=150,HIMASS,14
      IF(H(I).LT.S(I))S(I)=H(I)
    3 CONTINUE
      DO 4 I=109,HIMASS,14
      IF(HDI(I).LT.S(I))S(I)=HDI(I)
    4 CONTINUE
      DO 5 I=138,HIMASS,14
      IF(H(I).LT.S(I))S(I)=H(I)
    5 CONTINUE
      DO 6 I=139,HIMASS,14
      IF(HDI(I).LT.S(I))S(I)=HDI(I)
    6 CONTINUE
      DO 7 I=98,HIMASS,14
      IF(H(I).LT.S(I))S(I)=H(I)
    7 CONTINUE
```

```
      DO 8 I= 113, HIMASS, 14
      IF(HDI(I). LT. S(I))S(I)=HDI(I)
    8 CONTINUE
C
C  AN AROMATICS SPECTRUM IS OBTAINED BY SUBTRACTING CORRESPONDING ELE-
C    MENTS OF "S" FROM "H" FOR EVEN MASSES AND FROM "HDI" FOR ODD MASSES
C
      DO 9 I=191, HIMASS, 14
    9 A(I) = HDI(I)-S(I)
      DO 10 I=178, HIMASS, 14
   10 A(I) = H(I)-S(I)
      DO 11 I=179, HIMASS, 14
   11 A(I) = HDI(I)-S(I)
      DO 12 I=166, HIMASS, 14
   12 A(I) = H(I)-S(I)
      DO 13 I=167, HIMASS, 14
   13 A(I) = HDI(I)-S(I)
      DO 14 I=154, HIMASS, 14
   14 A(I) = H(I)-S(I)
      DO 15 I=141, HIMASS, 14
   15 A(I) = HDI(I)-S(I)
      DO 16 I=128, HIMASS, 14
   16 A(I) = H(I)
      DO 17 I=129, HIMASS, 14
   17 A(I) = HDI(I)
      DO 18 I=130, HIMASS, 14
   18 A(I) = H(I)
      DO 19 I=117, HIMASS, 14
   19 A(I) = HDI(I)
      DO 20 I=104, HIMASS, 14
   20 A(I) = H(I)
      DO 21 I=91, HIMASS, 14
   21 A(I) = HDI(I)
      DO 22 I=78, HIMASS, 14
   22 A(I) = H(I)
C
C  CORRECT THE "A" ARRAY FOR IRRELEVANT IONS AT MASSES 175, 176, 189, 190,
C    200, AND 213.
C
      C = (A(161) - A(203))/3. 0
      P = A(161) - C
      IF(P. LT. A(175))A(175)=P
      P = (A(175)+A(203))/2. 0
      IF(P. LT. A(189))A(189)=P
      C = (A(162) - A(204))/3. 0
      P = A(162) - C
      IF(P. LT. A(176))A(176)=P
      P = (A(176)+A(204))/2. 0
      IF(P. LT. A(190))A(190)=P
      P = (A(186)+A(214))/2. 0
      IF(P. LT. A(200))A(200)=P
      P = (A(199)+A(227))/2. 0
      IF(P. LT. A(213))A(213)=P

      IF(IFLAG4. EQ. 0)GO TO 507
      DO 400 I=1, HIMASS            ; 850726 SS CHECK FOR HIGH MASS
      J=HIMASS+1-I
      IF(S(J). GE. 0. 01) GO TO 410
  400 CONTINUE

  410 MAXS=J
      DO 420 I=1, HIMASS
      J=HIMASS+1-I
      IF(A(J). GE. 0. 01) GO TO 430
  420 CONTINUE
```

```
430 MAXA=J

500 FORMAT(//1H , 31X, 18HSATURATES SPECTRUM)
    WRITE(LUO, 501)((TITLE(J, I), I=1, 40), J=1, 2)   ;850710 TW TITLE CHANGE
    WRITE(LUO, 500)
501 FORMAT(1H1, 40A2/1X, 40A2)
    DO 502 I=31, MAXS, 7
    K = I + 6
    WRITE(LUO, 503)(J, J=I, K)
502 WRITE(LUO, 504)(S(J), J=I, K)
503 FORMAT(//, 1H , 7(I7, 3X))
504 FORMAT(1H , 7F10.2)
505 FORMAT(//1H , 31X, 18HAROMATICS SPECTRUM)
    WRITE(LUO, 501)((TITLE(J, I), I=1, 40), J=1, 2)   ;850710 TW TITLE CHANGE
    WRITE(LUO, 505)

    DO 506 I=31, MAXA, 7
    K = I + 6
    WRITE(LUO, 503)(J, J=I, K)
506 WRITE(LUO, 504)(A(J), J=I, K)

    NPASS = 1
507 CALL LOADIT("AROMAN")
    END
```

```
       PARAMETER HIMASS=758

      SUBROUTINE BSLINE (MSTART, CONST1, CONST2, ARRAY)

C
C    REVISION 1. 0 AS OF 260785
C             1. 1       860212
C

      COMMON /SASR/S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI
      DIMENSION ARRAY(HIMASS)

      MSTRT=MSTART+14
      DO 10 M=MSTART, HIMASS, 14
      IF (ARRAY(M))10, 11, 10
   10 CONTINUE

   11 MM=M-14
      IF (MM . LE. MSTRT) GO TO 21
      SLOPE = (CONST1*S(MSTART)-ARRAY(MM))/(CONST2-(1000. /FLOAT(MM))**2)
      B=CONST1*S(MSTART)-CONST2*SLOPE

      DO 20 M=MSTRT, MM, 14
   20 S(M)=SLOPE*(1000. /FLOAT(M))**2+B

      GO TO 25
   21 DO 22 M=MSTRT, 177, 14
   22 S(M)=ARRAY(M)

   25 RETURN
      END
```

```
C         SUBROUTINE AROMAN
C
C              OVERLAY AROMAN          CHAINED FROM SATARM (FIRST PASS )
C                                              OR FROM SATSAN (SECOND PASS )
C                                      CHAINS TO SATSAN


C
C     REVISION 1.0 AS OF 260785
C                  1.1       860212
C


C
C   THIS ROUTINE DETERMINES AROMATICS TYPE COMPOSITION FROM THE AROMATICS
C      SPECTRUM GENERATED BY SUBROUTINE "SATARM".  CALCULATIONS DESCRIBED I
C      ANAL CHEM 41, 1548(1969) REQUIRE SUPPLEMENTAL CORRECTIONS FOR THE
C      PRESENCE OF SATURATES. DATA FOR SATURATES ARE OBTAINED FROM SUB-
C      ROUTINE "SATSAN" AFTER A PRELIMINARY DETERMINATION OF THE MONO- AND
C      POLYAROMATICS. TWO CALCULATION PASSES ARE MADE.  A SECOND PASS THRU
C      THE SATURATES CALCULATIONS IN 'SATSAN' ARE ALSO MADE.
C
C      IF IFLAG4=1 SR(M) IS PRINTED AND
C        PEAK SUMS, BA(1-7), INVERSE RESULTS, BB(1-7),
C       AND CALCULATED DIVISIONS OF ALL COMPONENTS ARE PRINTED FOR
C       BOTH FIRST AND SECOND PASSES.
C


       PARAMETER HIMASS=758
       PARAMETER INPTLEN=6
       PARAMETER PARAMSIZE=1

       COMMON /AMATRIX/ AIN(7,7),BA(7),BB(7)

       COMMON /CDESC/
      1 METHODDESC(11),
      1 MENUDESC(11),
      1 KEEPDESC(11)

       COMMON /CDATA/ IDATA
       COMMON /CKEEP/ AKEEP(PARAMSIZE)

       INTEGER TITLE   ;850710 TW TITLE CHANGE.

       COMMON /MAIN/ TITLE(2,40), H(HIMASS), HDI(HIMASS), SUMH, SUMHDI,
      1IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

       COMMON /COMPON/ SUMSS, PAR, CPAR, CCP, CCP2, CCP3, SUMAA,
      1 A6A, A10S, A20A,  A8A, A22A, A36A,  A10A, A24A, A38A,
      1 A12A, A16S, A26A,  A14A, A28A, A42A,  A16A, A30A, A44A,
      1 A18A, A22S, A32A,  BL1, BL2, BL3, BL4, AMON, DITRI, NPASS,
      1 SA1, SA2, SA3, SA4, A6, A7, A8, A9, A10, A11, C1, C2, C3,
      1 AA6, AA8, AA10, AA12, AA14, AA16, AA18,
      1 A12, A13, A14, A15, A16, A17, A18, A19

       COMMON/SASR/S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI

       COMMON /CINPUT/ IDSW, INPUT, IFL, IBIT, IN(INPTLEN), FIN(INPTLEN)

       INTEGER DFSW, DFSW1, DFILE, SFILE

       COMMON /CMAIN/
      1 NPROG, DFSW, DFSW1, ITEMP(15),
      1 DFILE(12,6), SFILE(11,4),
      1 INSTD(3), IREFTABLE(11),
     1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISUB4,
     1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
     1 ISCN(45), IACQ(100), IDAT(45)

      EQUIVALENCE (AKEEP(1), AINF)

      DATA AIN/+1.8094, -0.1952, +0.0124, -0.0027, -0.0015, -0.0011, -0.0028,
     2          -0.1601, +2.0479, -0.2806, -0.0401, +0.0082, +0.0012, +0.0000,
     3          -0.0943, -0.2287, +2.3024, -0.4936, -0.0601, -0.0155, -0.0089,
     4          -0.0292, +0.0033, -0.0580, +1.9404, -0.1337, -0.0117, -0.0043,
     5          -0.0022, -0.0003, -0.0026, -0.0195, +1.9773, -0.1823, +0.0123,
     6          -0.0420, +0.0026, -0.0018, -0.0151, -0.0584, +2.0616, -0.4193,
     7          -0.2346, -0.1069, -0.0267, -0.0019, -0.0057, -0.0904, +1.9904/

      IF(AINF.EQ.0.0)AINF=1.0

      DO 2 I=1,7
      DO 2 J=1,7
    2 AIN(I,J) = AIN(I,J) * AINF

      IF(NPASS.EQ.2) GO TO 200      ;SS 850723 ADDED FOR CHAINING
C     THIS IS THE FIRST TIME THROUGH CODE

      DO 1 I=12,HIMASS
    1 SR(I) = 0.0

      PAR = 0.0
      CPAR = 0.0
      CCP = 0.0
      CCP2 = 0.0
      CCP3 = 0.0
      NPASS = 1
      BL1 = 0.0
      BL2 = 0.0
      BL3 = 0.0
      BL4 = 0.0
C
C     STORE NOMINAL PARENT-1 CONTRIBUTIONS IN "SR" ARRAY
C
      CALL BALINE   (105,.72,90.71,   147)
      CALL BALINE   (173,.66,34.12,   215)
      CALL BALINE   (185,1.0,29.22,   241)
      CALL BALINE   (183,.25,29.86,   197)
      CALL BALINE   (251,.64,15.87,   265)
      CALL BALINE   (277,.7,13.03,    291)
      CALL BALINE   (233,.58,18.42,   247)
C
C     SQUARE THE "SR" ARRAY AFTER SETTING SR(I) TO ZERO WHEN A(I) IS ZERO
C
      DO 28 I=78,HIMASS
      IF(A(I).EQ.0.0)SR(I)=0.0
   28 SR(I) = SR(I)*SR(I)
C
C     CORRECT CERTAIN PEAKS IN SR FOR DEVIATION FROM BASE LINE
C
      SR(147) = 1.44*SR(147)
      SR(197) = 3.1*SR(197)
      SR(211) = 2.52*SR(211)
      SR(225) = 2.07*SR(225)
      SR(239) = 1.83*SR(239)
      SR(253) = 1.59*SR(253)
      SR(267) = 1.39*SR(267)
      SR(281) = 1.28*SR(281)
      SR(295) = 1.26*SR(295)
      SR(309) = 1.14*SR(309)
      SR(323) = 1. 06*SR(323)
      SR(265) = 1. 42*SR(265)
      SR(279) = 1. 24*SR(279)
      SR(293) = 1. 12*SR(293)
      SR(307) = 1. 06*SR(307)
      SR(291) = 1. 24*SR(291)
      SR(305) = 1. 15*SR(305)
      SR(319) = 1. 07*SR(319)
      SR(333) = 1. 06*SR(333)
      SR(347) = 1. 05*SR(347)
      SR(361) = 1. 03*SR(361)
      SR(247) = 1. 61*SR(247)
      SR(261) = 1. 50*SR(261)
      SR(275) = 1. 44*SR(275)
      SR(289) = 1. 37*SR(289)
      SR(303) = 1. 28*SR(303)
      SR(317) = 1. 28*SR(317)
      SR(331) = 1. 21*SR(331)
      SR(345) = 1. 10*SR(345)
      SR(359) = 1. 09*SR(359)
      SR(373) = 1. 07*SR(373)
      SR(387) = 1. 05*SR(387)
C
C  IT IS NECESSARY THAT SR(M) IS LESS THAN OR EQUAL TO THE CORRESPONDING
C     VALUE FOR A(I)
C
      DO 29 I=78, HIMASS
      IF(A(I). LT. SR(I))SR(I)=A(I)
   29 CONTINUE

      IF(IFLAG4. EQ. 0)GO TO 504

      DO 490 I=1, HIMASS
      J=HIMASS+1-I
      IF(SR(J). GE. 0. 01) GO TO 495      ; FIND END OF ARRAY
  490 CONTINUE
  495 MAXMAS=J

      WRITE(LUO, 500)((TITLE(J, I), I=1, 40), J=1, 2)
  500 FORMAT(1H1, 2(40A2/1X)/1H , 36X, 8HSR ARRAY)
      DO 501 I=143, MAXMAS, 7
      K=I+6
      WRITE(LUO, 502)(J, J=I, K)
  501 WRITE(LUO, 503)(SR(J), J=I, K)
  502 FORMAT(//1H , 7(I7, 3X))
  503 FORMAT(1H , 7F10. 2)
C
C  ASSEMBLE GROUP SUMS FOR PROCESSING BY THE AIN MATRIX
C
  504 A6 = 0. 0
      DO 6 I=78, HIMASS, 14
    6 A6 = A6 + A(I)
      A7 = 0. 0
      DO 7 I=91, HIMASS, 14
    7 A7 = A7 + A(I)
      A6 = A6 + A7
      A8 = 0. 0
      DO 8 I=104, HIMASS, 14
    8 A8 = A8 + A(I)
      A9 = 0. 0
      DO 9 I=117, HIMASS, 14
    9 A9 = A9 + A(I)
      A8 = A8 + A9
      A10 = 0. 0
      DO 10 I=130, HIMASS, 14
   10 A10 = A10 + A(I)
```

```
      A11 = 0.0
      DO 11 I=129, HIMASS, 14
   11 A11 = A11 + A(I)
      A10 = A10 + A11
      A12 = 0.0
      DO 12 I=128, HIMASS, 14
    2 A12 = A12 + H(I)
      S12 = 0.0
      DO 9912 I=127, HIMASS, 14
  912 S12 = S12 + S(I)
      A12 = A12 -.26*S12
      A13 = 0.0
      DO 13 I=141, HIMASS, 14
   13 A13 = A13 + A(I)
      A12 = A12 + A13
      A14 = 0.0
      DO 14 I=154, HIMASS, 14
   14 A14 = A14 + A(I)
      A15 = 0.0
      DO 15 I=167, HIMASS, 14
   15 A15 = A15 + A(I)
      A14 = A14 + A15
      A16 = 0.0
      DO 16 I=166, HIMASS, 14
   16 A16 = A16 + A(I)
      A17 = 0.0
      DO 17 I=179, HIMASS, 14
   17 A17 = A17 + A(I)
      A16 = A16 + A17
      A18 = 0.0
      DO 18 I=178, HIMASS, 14
   18 A18 = A18 + A(I)
      A19 = 0.0
      DO 19 I=191, HIMASS, 14
   19 A19 = A19 + A(I)
      A18 = A18 + A19
C
C     CORRECT A6, A8, AND A10 FOR STERANE CONTRIBUTIONS AND STORE IN BA ARRAY
C
        C1 = 1.55*STIV + 3.41*STV + 2.17*STVI
        C2 = .101*STIV + 4.61*STV + 3.41*STVI
        C3 = .020*STIV + 0.30*STV + 4.61*STVI

  200 CALL SATINT(PAR, CPAR, CCP, CCP6, CCP8, CCP10, PAR7, CP7, SINT7,
     1S70L1, S70L2, CP9, SINT9, S90L1, S90L2, SINT11, S110L1, S110L2, PAR13,
     2A6, A7, A8, A9, A10, A11)

        BA(1) = A6 - C1 - PAR7 - CP7 - CCP6
        BA(2) = A8 - C2 - CP9 - CCP8
        BA(3) = A10 - C3 - CCP10
        BA(4) = A12 + BL1
        BA(5) = A14 + BL2
        BA(6) = A16 + BL3
        BA(7) = A18 + BL4

        IF(IFLAG4.EQ.0)GO TO 602

        WRITE(LUO,600)((TITLE(J,I),I=1,40),J=1,2),NPASS
  600 FORMAT('1',40A2/1X,40A2//1H ,7X,9HNPASS    =,I4)
      WRITE(LUO,601)(BA(I),I=1,7)
  601 FORMAT(//1X,7HBA(I)   ,7F9.1)

  602 DO 20 I=1,7
      IF(BA(I).LT.0.0)BA(I)=0.0
   CONTINUE
```

```
      DO 25 J=1, 7
      BB(J) = 0.0
      DO 24 I=1, 7
   24 BB(J) = BB(J) + BA(I)*AIN(J, I)

   25 CONTINUE

      DO 27 I=1, 7
      IF(BB(I). LT. 0. 0)BB(I)=0. 0
   27 CONTINUE

      IF(IFLAG4. EQ. 0)GO TO 701

      WRITE(LUO, 700)(BB(I), I=1, 7)
  700 FORMAT(1X, 7HBB(I)   , 7F9. 1)
  701 IF(NPASS. EQ. 2)GO TO 55

      AA6 = BB(1)
      AA8 = BB(2)
      AA10 = BB(3)
      AA12 = BB(4)
      AA14 = BB(5)
      AA16 = BB(6)
      AA18 = BB(7)

   55 AA7 = A7
      AA9 = A9
      AA11 = A11
      AA13 = A13
      AA15 = A15
      AA17 = A17
      AA19 = A19
C   RESOLVE OVERLAPPING TYPES IN THE 7 SERIES (Z=-6 TO Z=-18)
C   AND COMPUTE DIVISIONS OF COMPOUND TYPES.

      CALL RESOLVE(6, A6A, A10S, A20A, 91, 133, 147, 189, 0. 75, AA7, A6, A7,
     1 C1, AA6*0. 5578/AINF, PAR7, CP7, SINT7, S70L1, S70L2, BB(1))

      CALL RESOLVE(8, A8A, A22A, A36A, 117, 201, 215, 257, 0. 75, AA9, A8, A9,
     1 C2, AA8*0. 4997/AINF, 0. 0, CP9, SINT9, S90L1, S90L2, BB(2))

      CALL RESOLVE(10, A10A, A24A, A38A, 129, 227, 241, 283, 0. 75, AA11, A10, A11,
     1 C3, AA10*0. 4435/AINF, 0. 0, 0. 0, SINT11, S110L1, S110L2, BB(3))

      CALL RESOLVE(12, A12A, A16S, A26A, 141, 183, 197, 225, 0. 625, AA13,
     1 A12, A13, 0. 0, AA12*0. 5192/AINF, 0. 0, 0. 0, PAR13, 0. 0, PAR13, BB(4))

      CALL RESOLVE(14, A14A, A28A, A42A, 167, 251, 265, 307, 0. 75, AA15,
     1 A14, A15, 0. 0, AA14*0. 5075/AINF, 0. 0, 0. 0, 0. 0, 0. 0, 0. 0, BB(5))

      CALL RESOLVE(16, A16A, A30A, A44A, 179, 277, 291, 333, 0. 75, AA17,
     1 A16, A17, 0. 0, AA16*0. 4910/AINF, 0. 0, 0. 0, 0. 0, 0. 0, 0. 0, BB(6))

      CALL RESOLVE(18, A18A, A22S, A32A, 191, 233, 247, 289, 0. 75, AA19,
     1 A18, A19, 0. 0, AA18*0. 5073/AINF, 0. 0, 0. 0, 0. 0, 0. 0, 0. 0, BB(7))

C
C  THIS COMPLETES TYPE RESOLUTION.  TOTAL, MONO-, AND POLYAROMATICS ARE
C    NOW CALCULATED FOR USE IN SATURATES RESOLUTION
C
      SUMAA = 0. 0
      DO 104 I=1, 7
  104 SUMAA = SUMAA + BB(I)

               A6A + A8A + A10A
      DITRI = SUMAA - AMON
      IF(IFLAG4.EQ.0)GO TO 805

      WRITE(LUO,800)STIV,STV,STVI
  800 FORMAT(/1H ,2X,13HSTERANS DIV  ,5X,3F10.1)
      WRITE(LUO,802)SUMAA
  802 FORMAT(//,1H ,15HAROMATICS DIV  ,5X,F10.1)
      WRITE(LUO,803)A6A,A8A,A10A,A12A,A14A,A16A,A18A
  803 FORMAT(//,1X,7F10.1)
      WRITE(LUO,804)A10S,A22A,A24A,A16S,A28A,A30A,A22S
  804 FORMAT(1X,7F10.1)
      WRITE(LUO,804)A20A,A36A,A38A,A26A,A42A,A44A,A32A
  805 CONTINUE

      CALL LOADIT("SATSAN")
      END
```

```
       PARAMETER HIMASS=758

      SUBROUTINE BALINE(MSTART,CONST1,CONST2,MOLAP)


C
C    REVISION 1.0 AS OF 260785
C


C
C   THIS ROUTINE SETS UP BASELINES FOR RESOLVING OVERLAPPING AROMATICS
C
      COMMON/SASR/S(HIMASS),A(HIMASS),SR(HIMASS),AVMLWT,STIV,STV,STVI
      M1 = MOLAP + 14
      IF(A(MSTART).EQ.0.0)GO TO 21
      IF(A(MOLAP).EQ.0.0)GO TO 21
      IF(A(M1).EQ.0.0)GO TO 21

      DO 10 M=MSTART,HIMASS,14
      IF(AINT(A(M)))10,11,10
   10 CONTINUE

   11 MM = M - 14
      SLOPE = (((CONST1*A(MSTART))**0.5) - (A(MM))**0.5)/(CONST2 -(1000.
     1/FLOAT(MM))**2)
      B = (CONST1*A(MSTART))**0.5 - CONST2*SLOPE

      DO 20 M=MOLAP,MM,14
   20 SR(M) = SLOPE*(1000./FLOAT(M))**2 + B

   21 RETURN
      END
```

```
       PARAMETER HIMASS=758

      SUBROUTINE SATINT(PAR, CPAR, CCP, CCP6, CCP8, CCP10, PAR7, CP7,
     1SINT7, S7OL1, S7OL2, CP9, SINT9, S9OL1, S9OL2, SINT11, S11OL1, S11OL2,
     2PAR13, A6, A7, A8, A9, A10, A11)

C
C    REVISION 1. 0 AS OF 260785
C


C
C  THIS ROUTINE CALCULATES INTERFERENCE ON AROMATICS SUMMATIONS DUE TO
C     SATURATES
C
C   IT USES AVMLWT AND THE SUMS
C   IT RETURNS CORRECTED SUMS
C
      COMMON/SASR/S(HIMASS), A(HIMASS), SR(HIMASS), AVMLWT, STIV, STV, STVI

      F1 = . 00009*AVMLWT + . 0346
      CCP6 = F1*CCP
      F2 = . 00001542*AVMLWT + . 008133
      CCP8 = F2*CCP
      F3 = . 0000286*AVMLWT - . 003726
      CCP10 = F3*CCP
      CCP7 = . 0317*CCP
      CCP9 = CCP7*F2/F1
      CCP11 = CCP7*F3/F1
      CP7 = . 0023*CPAR
      CP9 = . 0005*CPAR
      F4 = . 00001675*AVMLWT - . 001615
      PAR13 = F4*PAR
      SINT7 = CCP6*A7/A6
      S7OL1 = (SINT7-CCP7)/2. 0
      IF(S7OL1. LT. 0. 0)S7OL1=0. 0
      S7OL2 = S7OL1
      SINT9 = CCP8*A9/A8
      S9OL1 = (SINT9-CCP9)/2. 0
      IF(S9OL1. LT. 0. 0)S9OL1=0. 0
      S9OL2 = S9OL1
      SINT11 = CCP10*A11/A10
      S11OL1 = (SINT11-CCP11)/2. 0
      IF(S11OL1. LT. 0. 0)S11OL1=0. 0
      S11OL2 = S11OL1
      PAR7 = . 001*PAR
      RETURN
      END
      PARAMETER HIMASS=758

      SUBROUTINE RESOLVE(IZ,S1,S2,S3,L1,L2,L3,L4,PARAM1,AA,A1,
     1 A2,CN,AB,P1,P2,P3,P4,P5,B)

C
C     REVISION 1.0 AS OF 260785
C



C          SUBROUTINE TO RESOLVE BASELINES
C          SEE AROMAN ORIGINAL
C
C          WRITTEN BY STEVE SIVERNS 850722
C
      COMMON /SASR/ S(HIMASS),A(HIMASS),SR(HIMASS),AVLMWT,STIV,STV,STVI

      S1=0.0
      DO 10 I=L1,L2,14
   10 S1=S1+A(I)

      DO 20 I=L3,HIMASS,14
   20 S1=S1+SR(I)

      S2=0.0
      DO 30 I=L3,L4,14
   30 S2=S2+A(I)-SR(I)

      S2=S2/PARAM1
      S3=AA-S1-S2
      ODDEVN=0.5
      IF(A1.GT.0.0) ODDEVN=A2/A1

      IF(S3)40,50,50
   40 S3=0.0
      S2=AA-S1
   50 TRASH=((A1-CN)-AB)*ODDEVN+P1+P2+P3+CN*ODDEVN
      IF(IZ.EQ.12)GO TO 100
   55 S1=S1-(TRASH-P4-P5-CN*ODDEVN*0.833)
      S2=S2-P4
      S3=S3-P5-CN*ODDEVN*0.833
      IF(IZ.GT.12)GO TO 200
      IF(S2.LT.0.0) S2=0.0
      IF(S3.LT.0.0) S3=0.0
   57 IF(S1.LT.0.0) S1=0.0
      SUMCL=S1+S2+S3
      IF(IZ.GT.12) GO TO 300
      IF(SUMCL) 60,60,70
   60 SUMCL=0.1
      S1=SUMCL
   70 S1=(S1/SUMCL)*B
      S2=(S2/SUMCL)*B
      S3=(S3/SUMCL)*B
      RETURN

  100 IF(P5.LE.S3) GO TO 55
      P5=S3
      P3=P5
      GO TO 55

 200  AA=AA-TRASH
      IF(AA.LT.1.0) AA=1.0
      GO TO 57
```

```
300 IF(S1.EQ.0.0) AA=S2+S3
    IF(AA.EQ.0.0) AA=1.0
    SUMCL=AA
    GO TO 70

    END
```

```
C        SUBROUTINE SATSAN  (PAR, CPAR, CCP2, CCP3, BL1, BL2, BL3, BL4, AMON, DITRI,
C       1NPASS, SA1, SA2, SA3, SA4)
C
C          OVERLAY SATSAN          CHAINED FROM AROMAN
C                                  CHAINS BACK TO AROMAN
C                                         OR TO REPORT
C
C                   THERE ARE TWO PASSES THROUGH THIS ROUTINE


C
C       REVISION 1.0 AS OF 260785
C                1.1       860210  ADDED COMMENTS AND HIMASS
C


C
C    THIS ROUTINE DETERMINES PARAFFINS, NONCONDENSED CYCLOPARAFFINS, AND
C      TWO CATEGORIES OF CONDENSED CYCLOPARAFFINS. PEAK SUMS FROM THE "S"
C      ARRAY ARE USED AFTER SUITABLE CORRECTIONS FOR AROMATICS ARE MADE.
C      TWO PASSES THRU THE PROGRAM ARE MADE.
C
C     IF IFLAG4 = 1, SATURATES PEAK SUMS, SA(1-4),
C       INVERSE RESULTS, SB(1-4), AND BASE LINE CORRECTIONS, BL1, BL2,
C       BL3, AND BL4 ARE PRINTED FOR EACH PASS.
C

        PARAMETER HIMASS=758
        PARAMETER INPTLEN=6
        PARAMETER PARAMSIZE=1

        COMMON /SMAT/ SM8(4,4),SM9(4,4),SM10(4,4),SM11(4,4),SM12(4,4),
       1SM13(4,4),SM14(4,4),SM15(4,4),SM16(4,4),SM17(4,4),SM18(4,4),
       2SM19(4,4),SM20(4,4),SM21(4,4),SM22(4,4),SM23(4,4),SM24(4,4),
       3SM25(4,4),SM26(4,4),SM27(4,4),SM28(4,4),SM29(4,4),SM30(4,4),
       4SM31(4,4),SM32(4,4),SM33(4,4),SM34(4,4),SM35(4,4),SM36(4,4),
       5SM37(4,4),SM38(4,4),SM39(4,4),SM40(4,4),SA(4),SB(4)

        COMMON /CDESC/
       1 METHODDESC(11),
       1 MENUDESC(11),
       1 KEEPDESC(11)

        COMMON /CDATA/ IDATA
        COMMON /CKEEP/ AKEEP(PARAMSIZE)

        INTEGER TITLE

        COMMON /MAIN/ TITLE(2,40),H(HIMASS),HDI(HIMASS),SUMH,SUMHDI,
       1 IFLAG1,IFLAG2,IFLAG3,IFLAG4,LUO

        COMMON /COMPON/ SUMSS,PAR,CPAR,CCP,CCP2,CCP3,SUMAA,
       1 A6A,A10S,A20A,  A8A,A22A,A36A,  A10A,A24A,A38A,
       1 A12A,A16S,A26A,  A14A,A28A,A42A,  A16A,A30A,A44A,
       1 A18A,A22S,A32A,  BL1,BL2,BL3,BL4,AMON,DITRI,NPASS,
       1 SA1,SA2,SA3,SA4,A6,A7,A8,A9,A10,A11,C1,C2,C3,
       1 AA6,AA8,AA10,AA12,AA14,AA16,AA18,
       1 A12,A13,A14,A15,A16,A17,A18,A19

        COMMON /SASR/ S(HIMASS),A(HIMASS),SR(HIMASS),AVMLWT,STIV,STV,STVI

        COMMON /CINPUT/ IDSW,INPUT,IFL,IBIT,IN(INPTLEN),FIN(INPTLEN)

        INTEGER DFSW,DFSW1,DFILE,SFILE
```

```
  COMMON /CMAIN/
 1 NPROG, DFSW, DFSW1, ITEMP(15),
 1 DFILE(12, 6), SFILE(11, 4),
 1 INSTD(3), IREFTABLE(11),
 1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISBU4,
 1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
 1 ISCN(45), IACQ(100), IDAT(45)

  DATA SM8/+2. 0804, -0. 2580, +0. 0252, +0. 0802,
 2         -0. 2017, +2. 2795, -0. 2228, -0. 7089,
 3         +0. 0144, -0. 1626, +3. 6900, -2. 9806,
 4         +0. 0000, -0. 0003, -0. 0153, +4. 1794/
  DATA SM9/+2. 0255, -0. 3055, +0. 0687, +0. 0630,
 2         -0. 2546, +2. 3236, -0. 5224, -0. 4791,
 3         +0. 0215, -0. 1961, +3. 3209, -2. 6629,
 4         +0. 0002, -0. 0021, -0. 0132, +4. 1784/
  DATA SM10/+2. 0292, -0. 3499, +0. 0847, +0. 0671,
 2          -0. 3046, +2. 3634, -0. 7735, -0. 2875,
 3          +0. 0238, -0. 1857, +3. 0633, -2. 4545,
 4          -0. 0009, +0. 0008, -0. 0753, +4. 2285/
  DATA SM11/+2. 0356, -0. 4006, +0. 1057, +0. 0700,
 2          -0. 3570, +2. 4144, -1. 0474, -0. 0819,
 3          +0. 0290, -0. 2082, +2. 9614, -2. 3715,
 4          -0. 0014, +0. 0043, -0. 1280, +4. 2884/
  DATA SM12/+2. 0439, -0. 4568, +0. 0885, +0. 1068,
 2          -0. 4033, +2. 4505, -1. 0453, -0. 0982,
 3          +0. 0336, -0. 2319, +2. 9440, -2. 3576,
 4          -0. 0018, +0. 0076, -0. 1825, +4. 3505/
  DATA SM13/+2. 0510, -0. 5066, +0. 0694, +0. 1424,
 2          -0. 4418, +2. 4898, -1. 0582, -0. 1030,
 3          +0. 0400, -0. 2609, +2. 9737, -2. 3709,
 4          -0. 0027, +0. 0138, -0. 2464, +4. 4012/
  DATA SM14/+2. 0588, -0. 5532, +0. 0536, +0. 1047,
 2          -0. 4812, +2. 5338, -1. 0732, -0. 0918,
 3          +0. 0455, -0. 2903, +2. 9971, -2. 3803,
 4          -0. 0036, +0. 0199, -0. 2982, +4. 4420/
  DATA SM15/+2. 0685, -0. 6058, +0. 0384, +0. 0726,
 2          -0. 5204, +2. 5837, -1. 1001, -0. 0714,
 3          +0. 0536, -0. 3288, +3. 0622, -2. 4212,
 4          -0. 0050, +0. 0284, -0. 3681, +4. 4970/
  DATA SM16/+2. 0767, -0. 6491, +0. 0245, +0. 0355,
 2          -0. 5653, +2. 6356, -1. 1368, -0. 0407,
 3          +0. 0631, -0. 3672, +3. 1410, -2. 4846,
 4          -0. 0067, +0. 0377, -0. 4378, +4. 5708/
  DATA SM17/+2. 0880, -0. 7003, +0. 0086, +0. 0109,
 2          -0. 6061, +2. 6959, -1. 1667, -0. 0437,
 3          +0. 0732, -0. 4097, +3. 2183, -2. 4674,
 4          -0. 0092, +0. 0509, -0. 5159, +4. 6205/
  DATA SM18/+2. 1005, -0. 7524, +0. 0011, -0. 0216,
 2          -0. 6474, +2. 7543, -1. 1992, -0. 0429,
 3          +0. 0854, -0. 4553, +3. 2901, -2. 4474,
 4          -0. 0129, +0. 0648, -0. 5901, +4. 6736/
  DATA SM19/+2. 1144, -0. 8056, -0. 0089, -0. 0485,
 2          -0. 6905, +2. 8154, -1. 2370, -0. 0393,
 3          +0. 0986, -0. 5018, +3. 3780, -2. 4371,
 4          -0. 0167, +0. 0814, -0. 6710, +4. 7281/
  DATA SM20/+2. 1268, -0. 8483, -0. 0238, -0. 0858,
 2          -0. 7352, +2. 8794, -1. 2HIMASS, -0. 0320,
 3          +0. 1142, -0. 5562, +3. 4558, -2. 4086,
 4          -0. 0211, +0. 1001, -0. 7444, +4. 7632/
  DATA SM21/+2. 1424, -0. 8912, -0. 0369, -0. 1259,
 2          -0. 7814, +2. 9426, -1. 3090, -0. 0243,
 3          +0. 1303, -0. 6077, +3. 5042, -2. 3651,
 4          -0. 0242, +0. 1110, -0. 7684, +4. 7637/
  DATA SM22/+2. 1478, -0. 9242, -0. 0536, -0. 1674,
 2          -0. 8169, +2. 9924, -1. 3387, -0. 0209,
     3         +0. 1437, -0. 6541, +3. 5512, -2. 3107,
     4         -0. 0269, +0. 1213, -0. 7872, +4. 7666/
      DATA SM23/+2. 1602, -0. 9675, -0. 0709, -0. 2027,
     2         -0. 8620, +3. 0770, -1. 3826, -0. 0169,
     3         +0. 1620, -0. 7098, +3. 5996, -2. 2607,
     4         -0. 0299, +0. 1308, -0. 7982, +4. 7655/
      DATA SM24/+2. 1764, -1. 0084, -0. 0827, -0. 2495,
     2         -0. 9101, +3. 1464, -1. 4208, -0. 0071,
     3         +0. 1810, -0. 7643, +3. 6475, -2. 2055,
     4         -0. 0334, +0. 1411, -0. 8080, +4. 7530/
      DATA SM25/+2. 1922, -1. 0412, -0. 1034, -0. 2915,
     2         -0. 9522, +3. 2167, -1. 4621, +0. 0046,
     3         +0. 1999, -0. 8227, +3. 7070, -2. 1721,
     4         -0. 0366, +0. 1515, -0. 8233, +4. 7657/
      DATA SM26/+2. 2126, -1. 0875, -0. 1168, -0. 3554,
     2         -0. 9998, +3. 3017, -1. 5021, +0. 0140,
     3         +0. 2240, -0. 8942, +3. 7740, -2. 1879,
     4         -0. 0433, +0. 1709, -0. 8631, +4. 9164/
      DATA SM27/+2. 2320, -1. 1249, -0. 1354, -0. 4098,
     2         -1. 0492, +3. 3783, -1. 5430, +0. 0350,
     3         +0. 2493, -0. 9633, +3. 8536, -2. 2792,
     4         -0. 0495, +0. 1899, -0. 9120, +5. 1179/
      DATA SM28/+2. 2519, -1. 1724, -0. 1416, -0. 4672,
     2         -1. 1024, +3. 4776, -1. 5959, +0. 0387,
     3         +0. 2845, -1. 0666, +3. 9492, -2. 3576,
     4         -0. 0588, +0. 2196, -0. 9668, +5. 3190/
      DATA SM29/+2. 2729, -1. 2222, -0. 1379, -0. 5384,
     2         -1. 1444, +3. 5560, -1. 6452, +0. 0449,
     3         +0. 3026, -1. 1192, +4. 0278, -2. 4554,
     4         -0. 0643, +0. 2380, -1. 0254, +5. 5673/
      DATA SM30/+2. 2935, -1. 2657, -0. 1372, -0. 6135,
     2         -1. 1964, +3. 6525, -1. 7029, +0. 0586,
     3         +0. 3358, -1. 2134, +4. 1277, -2. 5608,
     4         -0. 0743, +0. 2692, -1. 0901, +5. 8093/
      DATA SM31/+2. 3106, -1. 3083, -0. 1330, -0. 7039,
     2         -1. 2370, +3. 7423, -1. 7630, +0. 0754,
     3         +0. 3657, -1. 3038, +4. 2319, -2. 6844,
     4         -0. 0840, +0. 3008, -1. 1631, +6. 0919/
      DATA SM32/+2. 3300, -1. 3570, -0. 1249, -0. 8019,
     2         -1. 2801, +3. 8393, -1. 8301, +0. 0916,
     3         +0. 3984, -1. 4039, +4. 3493, -2. 8043,
     4         -0. 0956, +0. 3389, -1. 2438, +6. 3808/
      DATA SM33/+2. 3489, -1. 4102, -0. 0950, -0. 9185,
     2         -1. 3269, +3. 9498, -1. 9116, +0. 1112,
     3         +0. 4369, -1. 5196, +4. 4752, -2. 9412,
     4         -0. 1108, +0. 3843, -1. 3366, +6. 7199/
      DATA SM34/+2. 3724, -1. 4631, -0. 0799, -1. 0034,
     2         -1. 3796, +4. 0670, -1. 9840, +0. 0838,
     3         +0. 4785, -1. 6396, +4. 6054, -3. 0855,
     4         -0. 1280, +0. 4381, -1. 4454, +7. 1168/
      DATA SM35/+2. 3941, -1. 5146, -0. 0560, -1. 1365,
     2         -1. 4368, +4. 1819, -2. 0627, +0. 1061,
     3         +0. 5233, -1. 7643, +4. 7420, -3. 2428,
     4         -0. 1472, +0. 4961, -1. 5580, +7. 5122/
      DATA SM36/+2. 4166, -1. 5734, -0. 0186, -1. 2688,
     2         -1. 4912, +4. 3096, -2. 1574, +0. 1244,
     3         +0. 5711, -1. 9029, +4. 9001, -3. 4453,
     4         -0. 1687, +0. 5634, -1. 6935, +7. 9904/
      DATA SM37/+2. 4448, -1. 6404, +0. 0215, -1. 4023,
     2         -1. 5536, +4. 4490, -2. 2572, +0. 1358,
     3         +0. 6268, -2. 0587, +5. 0738, -3. 6723,
     4         -0. 1966, +0. 6474, -1. 8515, +8. 5329/
      DATA SM38/+2. 4756, -1. 7083, +0. 0621, -1. 5332,
     2         -1. 6263, +4. 5961, -2. 3510, +0. 1017,
     3         +0. 6929, -2. 2339, +5. 2550, -3. 8725,
     4         -0. 2294, +0. 7426, -2. 0224, +9. 0974/
```

```
      DATA SM39/+2.5038,-1.7836,+0.1160,-1.6941,
     2          -1.6930,+4.7519,-2.4584,+0.0745,
     3          +0.HIMASS9,-2.4204,+5.4585,-4.1241,
     4          -0.2686,+0.8605,-2.2332,+9.7905/
      DATA SM40/+2.5460,-1.8812,+0.1913,-1.8720,
     2          -1.7851,+4.9471,-2.5897,+0.0539,
     3          +0.8438,-2.6428,+5.6978,-4.4441,
     4          -0.3191,+1.0049,-2.4861,10.6097/
C
C  THE ORIGINAL BASE LINES USED IN OBTAINING THE "S" AND "A" SPECTRA ARE
C    IN ERROR BY AMOUNTS DEPENDING ON THE TOTAL QUANTITY OF AROMATICS
C    PRESENT IN THE SAMPLE.  CORRECTIONS TO SUMMATIONS FOR BOTH AROMATICS
C    AND SATURATES ARE MADE USING THE VALUE FOR TOTAL AROMATICS OBTAINED
C    IN THE FIRST PASS.
C
C  BEFORE MAKING THE ABOVE CORRECTIONS, SATURATES PEAK SUMS ARE OBTAINED
C
      IF(NPASS.EQ.2)GO TO 100          ; FIRST PASS CALCULATIONS
      S99 = 0.0
      II = 0

      DO 10 I=99,HIMASS,14
      II = II + 1
      S99 = S99 + S(I)
      IF(S(I))10,11,10
   10 CONTINUE

   11 II = II - 1
      I = I - 14
      S127 = S99 - S(113) - S(99)
      S141 = S127 - S(127)
      I127 = II - 2
      I141 = II - 3
      F = .15939E-3 + .8923E-6*AVMLWT
      FACTOR = ((AMON + DITRI)*F)/(S(99)-S(I))
      BL =  FACTOR*(S99 - FLOAT(II)*S(I))
      SA1 = S99 - BL + S(85) + S(71) + S(57) + S(43)
      BL1 = FACTOR*(S127 - FLOAT(I127)*S(I))*.26
      BL1 = BL1 + FACTOR*(S141 - FLOAT(I141)*S(I))
C
C  SA1 IS SUM FOR 43,HIMASS,14 AFTER BASE LINE CORRECTION.  BL1 IS CORRECTIO
C    TO AROMATICS SUM 128+

      TOTA = AMON + DITRI
      CALL BLINE  (84,154,5,SCPAR,.000948,TOTA,BLX)
      SA2 = SCPAR
      BL2 = BLX
      F = .32586E-3 + .17826E-5*AVMLWT
      CALL BLINE  (125,167,3,SCPAR,F,TOTA,BLX)
      SA2 = SA2 + SCPAR + S(111) + S(97) + S(83) + S(69) + S(55)
      BL2 = BL2 + BLX
C
C  SA2 IS SUM FOR 55+ PLUS 84+ CORRECTED FOR BASE LINE.  BL2 IS CORRECTIO
C    TO AROMATICS SUM 154+
C
      F = .15331E-3 + .10038E-5*AVMLWT
      CALL BLINE  (124,166,3,SCCP2,F,TOTA,BLX)
      SA3 = SCCP2 + S(110) + S(96)
      BL3 = BLX
      F = -.00129 + .171667E-4*AVMLWT
      CALL BLINE  (95,179,6,SCCP2,F,TOTA,BLX)
      SA3 = SA3 + SCCP2 + S(81)
      BL3 = BL3 + BLX
C
C  SA3 IS SUM 81+ PLUS 96+ CORRECTED.  BL3 IS CORRECTION TO AROMATICS 166
C
```

```
      F = .14725E-3 + .12375E-5*AVMLWT
      CALL BLINE  (136, 178, 3, SCCP3, F, TOTA, BLX)
      SA4 = SCCP3 + S(122) + S(108) + S(94)
      BL4 = BLX
      F = .356E-3 + .18667E-5*AVMLWT
      CALL BLINE  (149, 191, 3, SCCP3, F, TOTA, BLX)
      SA4 = SA4 + SCCP3 + S(135) + S(121) + S(107) + S(93)
      BL4 = BL4 + BLX
C
C  SA4 IS SUM 93+ PLUS 94+ CORRECTED. BL4 IS CORRECTION TO AROMATICS 178
C
C  ALL BASE LINE CORRECTIONS ARE COMPLETE. THE FOLLOWING SECTION APPLIES
C     CORRECTIONS TO THE SATURATES PEAK SUMS FOR MONOAROMATICS AND
C     POLYAROMATICS.
C
      IF(IFLAG4 .EQ. 0) GO TO 100
      WRITE(LUO, 501)S99
  501 FORMAT(//1H , 11HSUM S(I):  , 9X, F10.1)
      WRITE(LUO, 502)SA1, SA2, SA3, SA4
  502 FORMAT(1H , 8HSA(I):  , 12X, 4F10.1)
      WRITE(LUO, 503)BL1, BL2, BL3, BL4
  503 FORMAT(1H , 8HBL(I):  , 12X, 4F10.1)

C       2ND PASS CALCULATIONS PICK UP HERE

  100 FM = .0004146*AVMLWT - .06112
      FDT = .0002817*AVMLWT - .0538
      SA(1) = SA1 - FM*AMON - FDT*DITRI
      FM = .0003542*AVMLWT - .05476
      FDT = .0001288*AVMLWT - .01968
      SA(2) = SA2 - FM*AMON - FDT*DITRI
      FM = .0000558*AVMLWT - .00614
      FDT = .0000192*AVMLWT - .00296
      SA(3) = SA3 - FM*AMON - FDT*DITRI
      FM = .0000462*AVMLWT + .00268
      FDT = .0000135*AVMLWT - .00043
      SA(4) = SA4 - FM*AMON - FDT*DITRI

      DO 105 I=1, 4
  105 IF(SA(I).LT.0.0)SA(I)=0.0

C
C  CALCULATE AVERAGE CARBON NUMBER AND DEFINE SATURATES INVERSE MATRIX.
C
      NO = AVMLWT/14.0 + 0.5
      IF(NO-8)101, 102, 102
  101 NO = 8
  102 IF(NO-40)104, 104, 103
  103 NO = 40
  104 NMAT = NO - 7

      GO TO(108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122,
     1123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138,
     2139, 140), NMAT
C
C  DO INVERSE MATRIX MULTIPLICATION
C
  108 CALL SATMUL(SA, SB, SM8, $150)
  109 CALL SATMUL(SA, SB, SM9, $150)
  110 CALL SATMUL(SA, SB, SM10, $150)
  111 CALL SATMUL(SA, SB, SM11, $150)
  112 CALL SATMUL(SA, SB, SM12, $150)
  113 CALL SATMUL(SA, SB, SM13, $150)
  114 CALL SATMUL(SA, SB, SM14, $150)
  115 CALL SATMUL(SA, SB, SM15, $150)
  116 CALL SATMUL(SA, SB, SM16, $150)
```

```
 117 CALL SATMUL(SA, SB, SM17, $150)
 118 CALL SATMUL(SA, SB, SM18, $150)
 119 CALL SATMUL(SA, SB, SM19, $150)
 120 CALL SATMUL(SA, SB, SM20, $150)
 121 CALL SATMUL(SA, SB, SM21, $150)
 122 CALL SATMUL(SA, SB, SM22, $150)
 123 CALL SATMUL(SA, SB, SM23, $150)
 124 CALL SATMUL(SA, SB, SM24, $150)
 125 CALL SATMUL(SA, SB, SM25, $150)
 126 CALL SATMUL(SA, SB, SM26, $150)
 127 CALL SATMUL(SA, SB, SM27, $150)
 128 CALL SATMUL(SA, SB, SM28, $150)
 129 CALL SATMUL(SA, SB, SM29, $150)
 130 CALL SATMUL(SA, SB, SM30, $150)
 131 CALL SATMUL(SA, SB, SM31, $150)
 132 CALL SATMUL(SA, SB, SM32, $150)
 133 CALL SATMUL(SA, SB, SM33, $150)
 134 CALL SATMUL(SA, SB, SM34, $150)
 135 CALL SATMUL(SA, SB, SM35, $150)
 136 CALL SATMUL(SA, SB, SM36, $150)
 137 CALL SATMUL(SA, SB, SM37, $150)
 138 CALL SATMUL(SA, SB, SM38, $150)
 139 CALL SATMUL(SA, SB, SM39, $150)
 140 CALL SATMUL(SA, SB, SM40, $150)

 150 DO 141 I=1, 4
     IF(SA(I). EQ. 0. 0)SB(I)=0. 0
     IF(SB(I). LT. 0. 0)SB(I)=0. 0
 141 CONTINUE
C
C  MATRIX MULTIPLICATION COMPLETE
C
     PAR = SB(1)
     CPAR = SB(2)
     CCP2 = SB(3)
     CCP3 = SB(4)
     CCP=CCP2+CCP3
     SUMSS=PAR+CPAR+CCP

     IF(IFLAG4 . EQ.  0) GO TO 602
     WRITE(LUO, 500)NPASS
 500 FORMAT(//, 1H , 16HSATSAN NPASS    =, I4//)
     WRITE(LUO, 600)(SA(I), I=1, 4)
     WRITE(LUO, 601)(SB(I), I=1, 4)
 600 FORMAT(1H , 7HSA(I)  , 4F9. 1)
 601 FORMAT(1H , 7HSB(I)  , 4F9. 1)

 602 IF(NPASS . EQ.  2) CALL LOADIT("REPORT") ; ALL DONE
     NPASS = NPASS + 1
     CALL LOADIT("AROMAN")     ; DO SECOND PASS
     END
```

```
      PARAMETER HIMASS=758

      SUBROUTINE BLINE  ( MSTART, M2, IIDIFF, SSAT, F, TOTA, BLX)

C
C    REVISION 1.0 AS OF 260785
C             1.1       860210   ; ADDED HIMASS
C



C
C  THIS ROUTINE CALCULATES INTERFERENCE AT BASE LINE DUE TO AROMATICS
C
      COMMON/SASR/S(758),A(758),SR(758),AVMLWT,STIV,STV,STVI

      SSAT = 0.0
      SM2 = 0.0
      SUMSAT = 0.0
      BLX = 0.0
      II = 0

      DO 10 I = MSTART, 758, 14
      II = II + 1
      SUMSAT = SUMSAT + S(I)
      IF(S(I))10,11,10
   10 CONTINUE

   11 I = I - 14
      II = II - 1
      ISM2 = II - IIDIFF

      DO 20 M=M2,I,14
   20 SM2 = SM2 + S(M)

      FACTOR = (TOTA*F)/(S(MSTART) - S(I))
      BL = FACTOR*(SUMSAT - FLOAT(II)*S(I))
      SSAT = SUMSAT - BL
      BLX = FACTOR * (SM2 - FLOAT(ISM2)*S(I))
      RETURN
      END
      SUBROUTINE SATMUL(SA, SB, SMAT, DUM)

C
C    REVISION 1.0 AS OF 260785
C


C    850704 TW THE '*' WAS CHANGED TO VAR DUM TO ALLOW ABNORMAL
C      RETURNS.
C      THE RETURN STATEMENT AT THE END HAS ALSO BEEN CHANGED TO
C      RETURN DUM.
C
C
C   THIS ROUTINE PERFORMS INVERSE MATRIX MULTIPLICATION AND RETURNS
C   TO "SATSAN" AT STATEMANT 150.
C
      DIMENSION SA(4), SB(4), SMAT(4,4)

      DO 1 I=1,4
    1 SB(I) = 0.0

      DO 2 J=1,4
      DO 2 I=1,4
    2 SB(J) = SB(J) + SA(I)*SMAT(I,J)

      RETURN DUM
      END
```

```
C         SUBROUTINE REPORT(SUMSS, PAR, CPAR, CCP2, CCP3,
C        1SUMAA, A6A, A10S, A20A, A8A, A22A, A36A, A10A, A24A, A38A, A12A, A16S, A26A,
C        2A14A, A28A, A42A, A16A, A30A, A44A, A18A, A22S, A32A)

C           OVERLAY REPORT
C                                   CHAINED FROM SATSAN
C                                   CHAINS BACK TO ROBINS


C
C        REVISION 1.0 AS OF 260785
C                 1.1       860210  CLEANED UP A BIT
C


C
C      THIS ROUTINE PREPARES THE FINAL REPORT FOR THE PETROLEUM OIL ANALYSIS
C        BASIC INFORMATION IS IN VOLUME RATIOS. FROM THIS , VOLUME PERCENTS
C        ARE CALCULATED AND REPORTED.  IN ADDITION, WEIGHT PERCENTS ARE
C         REPORTED AS ESTIMATES.
C
          PARAMETER INPTLEN=6
          PARAMETER PARAMSIZE=1

          COMMON/DENS/ D(28, 18)

          COMMON /CDESC/
         1 METHODDESC(11),
         1 MENUDESC(11),
         1 KEEPDESC(11)

          COMMON /CDATA/ IDATA
          COMMON /CKEEP/ AKEEP(PARAMSIZE)

          INTEGER TITLE   ;850710 TW TITLE CHANGE.

          COMMON /MAIN/ TITLE(2, 40),  H(758),  HDI(758),  SUMH,  SUMHDI,
         1 IFLAG1, IFLAG2, IFLAG3, IFLAG4, LUO

          COMMON /COMPON/ SUMSS, PAR, CPAR, CCP, CCP2, CCP3, SUMAA,
         1 A6A, A10S, A20A,  A8A, A22A, A36A,  A10A, A24A, A38A,
         1 A12A, A16S, A26A,  A14A, A28A, A42A,  A16A, A30A, A44A,
         1 A18A, A22S, A32A,  BL1, BL2, BL3, BL4, AMON, DITRI, NPASS,
         1 SA1, SA2, SA3, SA4, A6, A7, A8, A9, A10, A11, C1, C2, C3,
         1 AA6, AA8, AA10, AA12, AA14, AA16, AA18,
         1 A12, A13, A14, A15, A16, A17, A18, A19

          COMMON/SASR/S(758), A(758), SR(758), AVMLWT, STIV, STV, STVI

          COMMON /CINPUT/ IDSW, INPUT, IFL, IBIT, IN(INPTLEN), FIN(INPTLEN)

          INTEGER DFSW, DFSW1, DFILE, SFILE

          COMMON /CMAIN/
         1 NPROG, DFSW, DFSW1, ITEMP(15),
         1 DFILE(12, 6), SFILE(11, 4),
         1 INSTD(3), IREFTABLE(11),
         1 IADD1, IADD2, ISUB1, ISUB2, ISUB3, ISUB4,
         1 JADD1, LIBRNAME, LIBRNUMB, IBUF,
         1 ISCN(45), IACQ(100), IDAT(45)

C
C      STORE TABLE OF DENSITIES
C
          DATA D /.68,.71,.72,.73,.74,.75,2*.76,2*.77,2*.78,4*.79,4*.80,6*
         2.81,2*.82,.76,.78,2*.79,2*.8,3*.81,8*.82,11*.83,
     36*. 88, 22*. 87,
     416*. 92, 7*. 91, 5*. 9,
     55*. 87, 8*. 86, 15*. 85,
     64*. 96, . 97, 2*. 95, . 94, 2*. 93, 2*. 92, 5*. 91, 7*. 9, 4*. 89,
     77*. 95, . 94, 2*. 93, 2*. 92, 5*. 91, 7*. 9, 4*. 89,
     86*1. 0, 1. 01, 1. 0, . 98, . 97, . 96, . 95, 2*. 94, 4*. 93, 6*. 92, 4*. 91,
     98*1. 08, 1. 06, 1. 03, 1. 01, 1. 0, . 99, . 98, . 97, 2*. 96, 3*. 95, 7*. 94, . 93,
     -9*1. 11, 1. 08, 1. 06, 1. 04, 1. 02, 1. 01, 1. 0, . 99, . 98, 4*. 97, 3*. 96, 4*. 95,
     110*1. 18, 1. 13, 1. 09, 1. 07, 1. 05, 1. 04, 1. 02, 2*1. 01, 1. 0, 2*. 99, 2*. 98, 2*. 97
     2, 3*. 96, 11*1. 23, 1. 19, 1. 16, 1. 13, 1. 11, 1. 09, 1. 08, 1. 06, 1. 05, 1. 04, 2*1. 03
     3, 2*1. 02, 1. 01, 2*1. 0, . 99, 13*1. 24, 1. 19, 1. 16, 1. 13, 1. 11, 1. 09, 1. 08, 1. 07,
     41. 06, 1. 05, 2*1. 04, 1. 03, 2*1. 02, 1. 01, 15*1. 25, 1. 21, 1. 17, 1. 15, 1. 13, 1. 12
     5, 1. 1, 1. 09, 1. 08, 1. 07, 2*1. 06, 2*1. 05, 18*1. 3, 1. 26, 1. 24, 1. 22, 1. 2, 1. 18,
     61. 17, 1. 16, 1. 15, 1. 14, 1. 13, 6*1. 16, 1. 15, 1. 13, 1. 11, 1. 09, 1. 07, 1. 05, 1. 04
     7, 1. 03, 4*1. 02, 4*1. 01, 4*1. 0, 2*. 99, 10*1. 24, 1. 22, 1. 2, 1. 18, 1. 16, 2*1. 14
     8, 2*1. 13, 2*1. 12, 3*1. 11, 3*1. 1, 2*1. 09, 15*1. 24, 1. 22, 1. 21, 1. 2, 1. 19, 1. 18
     9, 1. 17, 2*1. 16, 3*1. 15, 2*1. 14/
C
C  CALCULATE VOLUME PERCENTS OF COMPONENTS
C
      VAROM = 100. 0*SUMAA/SUMH
      VF = 100. 0/VAROM
      IF(VAROM. GT. 100. 0)VAROM = 100. 0
      VSATS = 100. 0 - VAROM
      IF(SUMSS. LE. 0. 0)SUMSS = 1. 0
      VPAR = PAR*VSATS/SUMSS
      VCPAR = CPAR*VSATS/SUMSS
      VCCP2 = CCP2*VSATS/SUMSS
      VCCP3 = CCP3*VSATS/SUMSS
      IF(VF. GT. 1. 0)VF=1. 0
      V6A = 100. 0*VF*A6A/SUMH
      V10S = 100. 0*VF*A10S/SUMH
      V20A = 100. 0*VF*A20A/SUMH
      V8A = 100. 0*VF*A8A/SUMH
      V22A = 100. 0*VF*A22A/SUMH
      V36A = 100. 0*VF*A36A/SUMH
      V10A = 100. 0*VF*A10A/SUMH
      V24A = 100. 0*VF*A24A/SUMH
      V38A = 100. 0*VF*A38A/SUMH
      V12A = 100. 0*VF*A12A/SUMH
      V16S = 100. 0*VF*A16S/SUMH
      V26A = 100. 0*VF*A26A/SUMH
      V14A = 100. 0*VF*A14A/SUMH
      V28A = 100. 0*VF*A28A/SUMH
      V42A = 100. 0*VF*A42A/SUMH
      V16A = 100. 0*VF*A16A/SUMH
      V30A = 100. 0*VF*A30A/SUMH
      V44A = 100. 0*VF*A44A/SUMH
      V18A = 100. 0*VF*A18A/SUMH
      V22S = 100. 0*VF*A22S/SUMH
      V32A = 100. 0*VF*A32A/SUMH
      VMONO = V6A + V8A + V10A
      VDI = V12A + V14A + V16A
      VTRI = V18A + V20A
      VTETRA = V22A + V24A
      VPENTA = V28A + V30A
      VSULF = V10S + V16S + V22S
      VUNID = V36A + V38A + V26A + V42A + V44A + V32A
      RECOV = 100. 0*(SUMAA + SUMSS)/SUMH
C
C  CALCULATE WEIGHT PERCENTS
C
      NO = AVMLWT/14. 0 + 0. 5
      L = NO - 6
      IF(L. LT. 1)L=1
      IF(L. GT. 28)L=28
      WPAR = VPAR*D(L, 1)
      WCPAR = VCPAR*D(L, 2)
      WCCP2 = VCCP2*D(L, 3)
      WCCP3 = VCCP3*D(L, 4)
      W6A = V6A*D(L, 5)
      W8A = V8A*D(L, 6)
      W10A = V10A*D(L, 7)
      W12A = V12A*D(L, 8)
      W14A = V14A*D(L, 9)
      W16A = V16A*D(L, 10)
      W18A = V18A*D(L, 11)
      W20A = V20A*D(L, 12)
      W22A = V22A*D(L, 13)
      W24A = V24A*D(L, 14)
      W28A = V28A*D(L, 15)
      W30A = V30A*D(L, 15)
      W36A = V36A*D(L, 15)
      W38A = V38A*D(L, 15)
      W26A = V26A*D(L, 15)
      W42A = V42A*D(L, 15)
      W44A = V44A*D(L, 15)
      W32A = V32A*D(L, 15)
      W10S = V10S*D(L, 16)
      W16S = V16S*D(L, 17)
      W22S = V22S*D(L, 18)
      SUMW = WPAR + WCPAR + WCCP2 + WCCP3 + W6A + W8A + W10A + W12A +
     1W14A + W16A + W18A + W20A + W22A + W24A + W28A + W30A + W36A + W38
     2A + W26A + W42A + W44A + W32A + W10S + W16S + W22S
      DENS = SUMW/100. 0
      WPAR = WPAR/DENS
      WCPAR = WCPAR/DENS
      WCCP2 = WCCP2/DENS
      WCCP3 = WCCP3/DENS
      W6A = W6A/DENS
      W8A = W8A/DENS
      W10A = W10A/DENS
      W12A = W12A/DENS
      W14A = W14A/DENS
      W16A = W16A/DENS
      W18A = W18A/DENS
      W20A = W20A/DENS
      W22A = W22A/DENS
      W24A = W24A/DENS
      W28A = W28A/DENS
      W30A = W30A/DENS
      W36A = W36A/DENS
      W38A = W38A/DENS
      W26A = W26A/DENS
      W42A = W42A/DENS
      W44A = W44A/DENS
      W32A = W32A/DENS
      W10S = W10S/DENS
      W16S = W16S/DENS
      W22S = W22S/DENS
      WSATS = WPAR + WCPAR + WCCP2 + WCCP3
      WAROM = 100. 0 - WSATS
      WMONO = W6A + W8A + W10A
      WDI = W12A + W14A + W16A
      WTRI = W18A + W20A
      WTETRA = W22A + W24A
      WPENTA = W28A + W30A
      WSULF = W10S + W16S + W22S
      WUNID = W36A + W38A + W26A + W42A + W44A + W32A
C
      WRITE(LUO, 201)((TITLE(J, I), I=1, 40), J=1, 2)
      WRITE(LUO, 200)
```

```
    WRITE(LUO, 217) AKEEP(1)
    WRITE(LUO, 202)SUMH, SUMHDI, DENS, RECOV, AVMLWT
    WRITE(LUO, 203)
    WRITE(LUO, 204)VSATS, WSATS, VPAR, WPAR, VCPAR, WCPAR, VCCP2, WCCP2,
   1VCCP3, WCCP3
    WRITE(LUO, 205)VAROM, WAROM, VMONO, WMONO
    WRITE(LUO, 206)V6A, W6A, V8A, W8A, V10A, W10A
    WRITE(LUO, 207)VDI, WDI, V12A, W12A, V14A, W14A, V16A, W16A
    WRITE(LUO, 208)VTRI, WTRI, V18A, W18A, V20A, W20A
    WRITE(LUO, 209)VTETRA, WTETRA, V22A, W22A, V24A, W24A
    WRITE(LUO, 210)VPENTA, WPENTA, V28A, W28A, V30A, W30A
    WRITE(LUO, 211)VSULF, WSULF, V10S, W10S, V16S, W16S, V22S,
   1W22S
    WRITE(LUO, 212)VUNID, WUNID, V36A, W36A, V38A, W38A, V26A,
   1W26A, V42A, W42A, V44A, W44A, V32A, W32A
200 FORMAT(1H , 20X, 40HMASS SPECTRAL ANALYSIS OF PETROLEUM OILS)
201 FORMAT(1H , 2(40A2/1H ))
202 FORMAT(//1H , 19HSUM OF PEAK HEIGHTS, 11X, F11. 1/
   11H , 24HSUM OF DE-ISOTOPED PEAKS, 6X, F11. 1/
   1/1H , 22HDENSITY OF TEST SAMPLE, 8X, F14. 4/
   1/1H , 18HAMOUNT OF RECOVERY, 12X, F11. 1/
   1//1H , 24HAVERAGE MOLECULAR WEIGHT, 6X, F11. 1
   1////45X, 1H*/45X, 12H*  ESTIMATED)
203 FORMAT(1H , 32X, 25HVOLUME PCT  *  WEIGHT PCT/
   132X, 27H------------ * ------------)
204 FORMAT(1H , 3X, 9HSATURATES, 24X, F7. 1, 8H *      , F7. 1/7X, 9HPARAFFINS,
   114X, F6. 1, 9X, 1H*, F5. 1/7X, 22HNONCOND CYCLOPARAFFINS, F7. 1, 9X, 1H*, F5. 1
   2/7X, 20HCOND CYCLOPAR 2-RING, F9. 1, 9X, 1H*, F5. 1/7X, 21HCOND CYCLOPAR 3
   3-RING+, F8. 1, 9X, 1H*, F5. 1)
205 FORMAT(1H , 3X, 9HAROMATICS, 24X, F7. 1, 8H *      , F7. 1      /5X, 5HMONO
   1-, 20X, F10. 1, 5X, 1H*, F9. 1)
206 FORMAT(1H , 6X, 8HBENZENES, 15X, F6. 1, 9X, 1H*, F5. 1       /7X, 17HNAPHTHEN
   1EBENZENES, F12. 1, 9X, 1H*, F5. 1       /7X, 19HDINAPHTHENEBENZENES, F10. 1,
   29X, 1H*, F5. 1)
207 FORMAT(1H , 4X, 3HDI-, 25X, F7. 1, 5X, 1H*, F9. 1       /7X, 12HNAPHTHALENES,
   1F17. 1, 9X, 1H*, F5. 1       /7X, 23HACENAPHTHENES, DBZFURANS, F6. 1, 9X, 1H*,
   2F5. 1       /7X, 9HFLUORENES, F20. 1, 9X, 1H*, F5. 1)
208 FORMAT(1H , 4X, 4HTRI-, 24X, F7. 1, 5X, 1H*, F9. 1       /7X, 13HPHENANTHRENE
   1S, F16. 1, 9X, 1H*, F5. 1       /7X, 22HNAPHTHENEPHENANTHRENES, F7. 1, 9X, 1H*
   2, F5. 1)
209 FORMAT(1H , 4X, 6HTETRA-, 22X, F7. 1, 5X, 1H*, F9. 1       /7X, 7HPYRENES,
   113X, F9. 1, 9X, 1H*, F5. 1       /7X, 9HCHRYSENES, 11X, F9. 1, 9X, 1H*, F5. 1)
210 FORMAT(1H , 4X, 6HPENTA-, 22X, F7. 1, 5X, 1H*, F9. 1       /7X, 9HPERYLENES,
   111X, F9. 1, 9X, 1H*, F5. 1       /7X, 17HDIBENZANTHRACENES, F12. 1, 9X, 1H*,
   2F5. 1)
211 FORMAT(1H , 4X, 10HTHIOPHENO-, 17X, F8. 1, 5X, 1H*, F9. 1       /7X, 15HBENZO
   1THIOPHENES, F14. 1, 9X, 1H*, F5. 1       /7X, 17HDIBENZOTHIOPHENES, F12. 1,
   29X, 1H*, F5. 1       /7X, 22HNAPHTHOBENZOTHIOPHENES, F7. 1, 9X, 1H*, F5. 1)
212 FORMAT(1H , 4X, 12HUNIDENTIFIED, 15X, F8. 1, 5X, 1H*, F9. 1       /7X, 24HCLA
   1SS I  WITH NAPHPHENAN, 14X, 1H*/7X, 8HCLASS II, 12X, F9. 1, 9X, 1H*, F5. 1,
   2     /7X, 9HCLASS III, 11X, F9. 1, 9X, 1H*, F5. 1       /7X, 8HCLASS IV, 12X,
   3F9. 1, 9X, 1H*, F5. 1       /7X, 7HCLASS V, 13X, F9. 1, 9X, 1H*, F5. 1      /7X,
   48HCLASS VI, 12X, F9. 1, 9X, 1H*, F5. 1       /7X, 9HCLASS VII, 11X, F9. 1, 9X,
   51H*, F5. 1)
    TSTPK1 = H(135) + H(163)
    IF(H(149). GT. TSTPK1)WRITE(LUO, 215)
215 FORMAT(//, 10X, 42HWARNING - PEAK AT MASS 149 ABNORMALLY HIGH, /
   112X, 58HMAY INDICATE CONTAMINATION OF SAMPLE WITH PHTHALATE ESTERS,
   2/12X, 33HMAY CAUSE ERRORS IN THIS ANALYSIS)
    WRITE (LUO, 216)
216 FORMAT (1H1)
217 FORMAT (" AIN FACTOR", 25X, F10. 5/)
    CALL LOADIT("ROBINS")
    END
```

Enclosed is a printout of the full results of the file TESTFILE included on the tape. These results can be used to verify operation of the program should changes be made. The output was produced with the following commands:

```
R;H;L;T;A200;E
```

The standard short printout could be obtained with the commands:

```
H;G200;E
```

```
SHELLA3SS.MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

          SUM OF POLY AND MONO PEAKS FOR THIS TABLE:    13114300.  11967400.

                 MASS SPECTRUM:  TOP-POLYISOTOPIC, BOTTOM-MONOISOTOPIC


       17          18          19          20          21          22          23
     3083.9     19423.9       234.9      5215.9       550.9      1589.9       524.9
     3053.14    19357.90        0.00     5213.73      438.26     1579.91      490.78

       24          25          26          27          28          29          30
      571.9      1119.9      2111.9     51007.9         0.0    116991.0      4091.9
      561.20     1107.80     2087.81    50962.00        0.00   116985.00     1474.80

       31          32          33          34          35          36          37
      358.9         0.0       720.9      1867.9       447.9      2041.9       879.9
      310.18        0.00      720.89     1844.61      387.92     2028.77      814.06

       38          39          40          41          42          43          44
     1515.9     59967.9     18111.9    344063.0     81663.9    609279.0     37439.9
     1488.76    59918.90    16141.10   343508.00    70259.30   606809.00    17095.50

       45          46          47          48          49          50          51
     3451.9      1317.9      1245.9      1537.9       620.9      3995.9     19583.9
     2643.30     1197.02     1192.38     1485.59      555.92     3970.83    19410.60

       52          53          54          55          56          57          58
     8559.9     47039.9     32287.9    502783.0    233983.0    815103.0     42559.9
     7709.02    46688.00    30228.30   501415.00   211751.00   805318.00     6488.02

       59          60          61          62          63          64          65
     8431.9      1409.9      1575.9      2251.9     12271.9      9055.9     42111.9
     7529.27      998.02     1513.25     2168.80    12152.30     8391.06    41638.80

       66          67          68          69          70          71          72
    17151.9    176383.0     74239.9    444415.0    215807.0    469503.0     28799.9
    14859.80   175516.00    64550.00   440633.00   191314.00   458327.00     3029.53

       73          74          75          76          77          78          79
     4567.9      2639.9      4567.9      6439.9     78207.9     27455.9     78591.9
     3821.64     2387.69     4405.66     6148.00    77797.60    22340.20    76982.40

       80          81          82          83          84          85          86
    27583.9    254975.0    135423.0    297471.0    120319.0    269311.0     19679.9
    22469.10   253351.00   118606.00   289133.00   100868.00   262049.00     1982.15

       87          88          89          90          91          92          93
     4127.9      2279.9     14447.9      4535.9    189183.0     40831.9     45887.9
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  3502.23   2009.63  14285.90   3439.14 188884.00  26330.70  43385.00

     94        95        96        97        98        99       100
 25791.9  237823.0  115071.0  275967.0   80767.9   69631.9    7127.9
 22383.10 235985.00  96766.30 267861.00  59723.80  64289.30   1961.91

    101       102       103       104       105       106       107
  5543.9   11247.9   38527.9   31903.9  307711.0   76799.9   39295.9
  5221.91  10787.20  37567.80  28579.20 305079.00  49905.90  33870.50

    108       109       110       111       112       113       114
 20831.9  147711.0   69247.9  162303.0   57663.9   52031.9    5007.9
 17676.80 146035.00  56272.20 156816.00  43553.90  47616.40    616.62

    115       116       117       118       119       120       121
 85375.9   29055.9  101759.0   36159.9  264191.0  109951.0   40127.9
 85154.40  20678.90  99356.00  26269.10 261165.00  83995.40  30662.90

    122       123       124       125       126       127       128
 16927.9   88447.9   39167.9   85119.9   40959.9   48255.9   60927.9
 13516.40  86969.40  30450.60  81698.80  32667.10  44625.00  56312.60

    129       130       131       132       133       134       135
 50815.9   22815.9  108927.0   38591.9  113791.0   81151.9   41599.9
 44967.50  17640.20 106751.00  26779.30 110267.00  68869.70  33406.40

    136       137       138       139       140       141       142
 16079.9   57983.9   26559.9   42175.9   27391.9   70527.9   39935.9
 12015.20  56472.20  20244.40  39619.90  22883.30  67764.60  32268.60

    143       144       145       146       147       148       149
 33919.9   17439.9   90239.9   38911.9   47871.9   44479.9   42047.9
 29945.10  13648.00  88393.90  28137.00  43877.90  38975.30  37025.50

    150       151       152       153       154       155       156
 15583.9   48127.9   40319.9   36607.9   27007.9   51071.9   32831.9
 10824.60  46562.10  34576.90  32077.00  22857.50  48059.90  26794.80

    157       158       159       160       161       162       163
 28511.9   14783.9   56959.9   30239.9   32511.9   27263.9   31871.9
 24900.10  11321.20  55269.00  22855.00  29049.40  23237.70  28560.70

    164       165       166       167       168       169       170
 13375.9   58687.9   27487.9   34111.9   20799.9   38463.9   25503.9
  9401.87  57209.00  19809.70  31011.70  16508.30  36009.60  20562.20

    171       172       173       174       175       176       177
 24543.9   12255.9   34623.9   21663.9   26911.9   21439.9   24831.9
 21500.60   9016.67  33132.20  16837.70  24186.00  17811.90  22044.90

    178       179       180       181       182       183       184
 25727.9   39423.9   22143.9   31359.9   20671.9   27903.9   19647.9
 22390.30  35992.40  16746.70  28600.20  16383.90  25261.40  15836.90
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   185        186        187        188        189        190        191
21759. 9   11151. 9   23103. 9   15535. 9   30015. 9   16767. 9   28223. 9
19222. 80   8039. 66  21653. 50  12108. 10  27907. 30  12321. 80  26008. 10

   192        193        194        195        196        197        198
19327. 9   30367. 9   20095. 9   31071. 9   19615. 9   24095. 9   14287. 9
15164. 50  27727. 80  15625. 60  28335. 20  15037. 00  21437. 90  10780. 30

   199        200        201        202        203        204        205
18751. 9   11951. 9   17663. 9   19455. 9   21151. 9   13263. 9   20095. 9
16829. 50   9052. 76  15954. 40  16702. 90  18184. 20  10038. 40  18198. 50

   206        207        208        209        210        211        212
15279. 9   26111. 9   18367. 9   24607. 9   16159. 9   20767. 9   12031. 9
12131. 40  23862. 80  14244. 90  21929. 40  12323. 70  18429. 20   8797. 36

   213        214        215        216        217        218        219
16223. 9   10351. 9   21151. 9   13423. 9   16063. 9   12303. 9   16015. 9
14514. 80   7680. 63  19586. 50   9856. 27  14037. 10   9678. 83  14097. 90

   220        221        222        223        224        225        226
11487. 9   18975. 9   13519. 9   16991. 9   11583. 9   16447. 9   12207. 9
 8849. 93  17200. 20  10339. 30  14902. 60   8783. 72  14665. 20   9468. 07

   227        228        229        230        231        232        233
12367. 9   11263. 9   15999. 9   11887. 9   13567. 9   11327. 9   12671. 9
10463. 50   9163. 56  14109. 80   9090. 09  11627. 80   8992. 78  10787. 80

   234        235        236        237        238        239        240
 9119. 9   14447. 9    9759. 9   12175. 9    8255. 9   14703. 9    8159. 9
 6940. 43  12960. 90   7201. 53  10600. 60   6134. 35  13367. 00   5529. 79

   241        242        243        244        245        246        247
 9551. 9    9503. 9   12223. 9   11663. 9   12095. 9    9855. 9   10591. 9
 8280. 27   7768. 15  10527. 80   9427. 78  10025. 10   7685. 13   8874. 04

   248        249        250        251        252        253        254
 8575. 9   10303. 9    7775. 9    8831. 9    7079. 9    9727. 9    5743. 9
 6663. 62   8808. 46   5892. 82   7489. 10   5472. 01   8491. 92   3940. 67

   255        256        257        258        259        260        261
 6623. 9    6839. 9    8167. 9    8895. 9    9023. 9    8367. 9    7847. 9
 5673. 52   5576. 72   6880. 90   7336. 34   7340. 29   6672. 62   6291. 55

   262        263        264        265        266        267        268
 8127. 9    8367. 9    5999. 9    7327. 9    5335. 9    7759. 9    4831. 9
 6664. 49   6832. 84   4420. 33   6252. 12   3923. 74   6799. 48   3312. 47

   269        270        271        272        273        274        275
 5479. 9    4087. 9    5983. 9    5999. 9    5999. 9    6471. 9    5911. 9
 4635. 52   2995. 19   5215. 55   4778. 57   4822. 71   5294. 22   4627. 96
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  276          277          278          279          280          281          282
5431. 9      6335. 9      4783. 9      5991. 9      3695. 9      8559. 9      4583. 9
4283. 56     5278. 58     3513. 17     5088. 71     2483. 54     7888. 57     2771. 39

  283          284          285          286          287          288          289
5343. 9      3471. 9      4687. 9      4495. 9      4799. 9      4663. 9      5287. 9
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  290          291          292          293          294          295          296
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  304          305          306          307          308          309          310
3811. 9      4615. 9      3831. 9      4135. 9      3435. 9      4599. 9      3507. 9
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3735. 9      3119. 9      3679. 9      3159..9      3971. 9      3499. 9      4143. 9
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  318          319          320          321          322          323          324
3499. 9      4279. 9      3651. 9      3815. 9      3315. 9      4055. 9      3295. 9
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4087. 9      2547. 9      3839. 9      3247. 9      3355. 9      3483. 9      3547. 9
3377. 97     1578. 50     3307. 55     2317. 17     2629. 09     2707. 27     2739. 44

  332          333          334          335          336          337          338
3595. 9      3575. 9      3387. 9      3715. 9      3367. 9      3739. 9      3119. 9
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3703. 9      2871. 9      3575. 9      2987. 9      3259. 9      3375. 9      3283. 9
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  346          347          348          349          350          351          352
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3355. 9      2395. 9      4591. 9      3291. 9      3451. 9      3315. 9      2931. 9
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  360          361          362          363          364          365          366
3195. 9      3139. 9      2967. 9      3203. 9      3059. 9      3771. 9      3135. 9
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  374       375       376       377       378       379       380
 3179.9    2631.9    2943.9    2583.9    3207.9    3067.9    2751.9
 2478.88   1804.28   2296.33   1817.69   2563.46   2220.12   1974.32


  381       382       383       384       385       386       387
 2767.9    2727.9    2743.9    2867.9    3443.9    3307.9    3195.9
 2078.61   1998.85   2029.01   2146.96   2684.61   2376.02   2334.28


  388       389       390       391       392       393       394
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 1801.10   2280.14   1735.77   2050.21   1893.47   2167.15   2028.91


  395       396       397       398       399       400       401
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 1798.74   2096.32   1666.29   2077.07   2338.26   2413.51   2151.85


  402       403       404       405       406       407       408
 2375.9    2703.9    2683.9    1895.9    2863.9    2243.9    2555.9
 1563.74   2093.52   1932.14   1169.17   2390.60   1415.04   1979.78


  409       410       411       412       413       414       415
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 1594.35   1815.57   1532.63   1594.42   1896.67   2024.62   1909.57


  416       417       418       419       420       421       422
 2475.9    2235.9    2375.9    2267.9    1961.9    2207.9    2095.9
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  423       424       425       426       427       428       429
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  437       438       439       440       441       442       443
 1585.9    2055.9    1299.9    2163.9    1551.9    2013.9    1865.9
 1019.36   1614.26    666.53   1829.75    863.05   1596.58   1247.14


  444       445       446       447       448       449       450
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  451       452       453       454       455       456       457
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SHELLA3SS.MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

                              SATURATES SPECTRUM

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      94         95         96         97         98         99        100
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     108        109        110        111        112        113        114
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     115        116        117        118        119        120        121
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     122        123        124        125        126        127        128
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     136       137       138       139       140       141       142
15733.10  51572.80  20365.70  23962.50  22737.80  14215.00      0.00

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    0.00      0.00      0.00      0.00      0.00      0.00  28959.30

     150       151       152       153       154       155       156
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     157       158       159       160       161       162       163
    0.00      0.00      0.00      0.00      0.00      0.00  24701.70

     164       165       166       167       168       169       170
10956.20  28558.20  12820.90  11046.20  15076.60  10366.20      0.00

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    0.00      0.00      0.00      0.00      0.00      0.00  19334.90

     178       179       180       181       182       183       184
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     192       193       194       195       196       197       198
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     213       214       215       216       217       218       219
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     220       221       222       223       224       225       226
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     227       228       229       230       231       232       233
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     234       235       236       237       238       239       240
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     241       242       243       244       245       246       247
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2, 81, 2*, 82, . 76, . 78, 2*, 79, 2*, 8, 3*, 81, 8*, 82, 11*, 83,
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    248        249        250        251        252        253        254
 5424. 96   7596. 85   6458. 09   3049. 15   7032. 74   4786. 47      0. 00

    255        256        257        258        259        260        261
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    262        263        264        265        266        267        268
 4851. 31   6687. 14   5761. 57   2570. 22   5335. 99   4276. 76      0. 00

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    276        277        278        279        280        281        282
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    283        284        285        286        287        288        289
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   3561. 15

    290        291        292        293        294        295        296
 3943. 17   4211. 91   4067. 99   1798. 61   3907. 99   3466. 41      0. 00

    297        298        299        300        301        302        303
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   2893. 02

    304        305        306        307        308        309        310
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    311        312        313        314        315        316        317
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   2292. 37

    318        319        320        321        322        323        324
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    325        326        327        328        329        330        331
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   1996. 65

    332        333        334        335        336        337        338
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    339        340        341        342        343        344        345
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   1736. 19

    346        347        348        349        350        351        352
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    353        354        355        356        357        358        359
    0. 00      0. 00      0. 00      0. 00      0. 00      0. 00   1505. 61

    360        361        362        363        364        365        366
 2527. 16   2186. 00   2929. 50   1093. 19   2984. 08   2193. 33      0. 00
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   402       403       404       405       406       407       408
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   444       445       446       447       448       449       450
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   451       452       453       454       455       456       457
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   458       459       460       461       462       463       464
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   465       466       467       468       469       470       471
     0.00      0.00      0.00      0.00      0.00      0.00    338.75

   472       473       474       475       476       477       478
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   500         501         502         503         504         505         506
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1007. 13     158. 31     856. 99     457. 73     831. 96     451. 64       0. 00

   563         564         565         566         567         568         569
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   584         585         586         587         588         589         590
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   591         592         593         594         595         596         597
    0. 00       0. 00       0. 00       0. 00       0. 00       0. 00       0. 00
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598      599      600      601      602      603      604
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605      606      607      608      609      610      611
  0.00     0.00     0.00     0.00     0.00     0.00     0.00

612      613      614      615      616      617      618
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619      620      621      622      623      624      625
  0.00     0.00     0.00     0.00     0.00     0.00     0.00

626      627      628      629      630      631      632
703.99   137.39   781.13     0.00   501.51   456.50     0.00

633      634      635      636      637      638      639
  0.00     0.00     0.00     0.00     0.00     0.00     0.00

640      641      642      643      644      645      646
737.99   104.41   734.99     0.00   447.99   563.19     0.00
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SHELLA3SS.MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

                                  AROMATICS SPECTRUM

      31         32         33         34         35         36         37
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      38         39         40         41         42         43         44
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      45         46         47         48         49         50         51
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      52         53         54         55         56         57         58
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      59         60         61         62         63         64         65
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      66         67         68         69         70         71         72
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      73         74         75         76         77         78         79
       0.00       0.00       0.00       0.00       0.00   27455.90       0.00

      80         81         82         83         84         85         86
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

      87         88         89         90         91         92         93
       0.00       0.00       0.00       0.00  188884.00   40831.90       0.00

      94         95         96         97         98         99        100
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

     101        102        103        104        105        106        107
       0.00       0.00       0.00   31903.90  305079.00   76799.90       0.00

     108        109        110        111        112        113        114
       0.00       0.00       0.00       0.00       0.00       0.00       0.00

     115        116        117        118        119        120        121
       0.00       0.00   99356.00   36159.90  261165.00  109951.00       0.00

     122        123        124        125        126        127        128
       0.00       0.00       0.00       0.00       0.00       0.00   60927.90

     129        130        131        132        133        134        135
   44967.50   22815.90  106751.00   38591.90  110267.00   81151.90       0.00
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     136        137        138        139        140        141        142
    0.00       0.00       0.00       0.00       0.00   53549.60   39935.90

     143        144        145        146        147        148        149
29945.10   17439.90   88393.90   38911.90   43877.90   44479.90       0.00

     150        151        152        153        154        155        156
    0.00       0.00       0.00       0.00    9942.37   36420.10   32831.90

     157        158        159        160        161        162        163
24900.10   14783.90   55269.00   30239.90   29049.40   27263.90       0.00

     164        165        166        167        168        169        170
    0.00       0.00   14667.00   19965.40    5723.35   25643.30   25503.90

     171        172        173        174        175        176        177
21500.60   12255.90   33132.20   21663.90   24186.00   21439.90       0.00

     178        179        180        181        182        183        184
16662.20   14072.90   10691.20   19772.30    6508.08   15926.20   19647.90

     185        186        187        188        189        190        191
19222.80   11151.90   21653.50   15535.90   21185.10   16767.90    8719.86

     192        193        194        195        196        197        198
11446.70    9102.10    9836.06   20730.90    7505.52   13410.50   14287.90

     199        200        201        202        203        204        205
16829.50   10751.90   15954.40   19455.90   18184.20   13263.90    7089.58

     206        207        208        209        210        211        212
 8404.31   10660.50    9288.78   16734.10    5706.13   11458.00   12031.90

     213        214        215        216        217        218        219
13646.50   10351.90   19586.50   13423.90   14037.10   12303.90    4730.20

     220        221        222        223        224        225        226
 5261.67    6874.53    5252.88   10776.20    2485.94    8559.27   12207.90

     227        228        229        230        231        232        233
10463.50   11263.90   14109.80   11887.90   11627.80   11327.90    3483.58

     234        235        236        237        238        239        240
 3320.59    4097.10    2477.78    6948.20     281.61    7978.67    8159.99

     241        242        243        244        245        246        247
 8280.27    9503.99   10527.80   11663.90   10025.10    9855.99    2613.33
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  248        249        250        251        252        253        254
3151.03    1211.61    1317.90    4439.94      47.25    3705.45    5743.99

  255        256        257        258        259        260        261
5673.52    6839.99    6880.90    8895.99    7340.29    8367.99    1065.54

  262        263        264        265        266        267        268
3276.68     145.69     238.42    3681.89       0.00    2522.71    4831.99

  269        270        271        272        273        274        275
4635.52    4087.99    5215.55    5999.99    4822.71    6471.99     398.75

  276        277        278        279        280        281        282
1069.27     100.32       0.00    2974.63       0.00    4047.23    4583.99

  283        284        285        286        287        288        289
4541.48    3471.99    4025.85    4495.99    3883.76    4663.99     773.39

  290        291        292        293        294        295        296
 232.82     240.94       0.00    2350.29       0.00     989.60    3835.99

  297        298        299        300        301        302        303
3340.26    3171.99    3397.48    3679.99    3345.46    4191.99     392.78

  304        305        306        307        308        309        310
 231.75     402.99       0.00    1808.56       0.00     742.50    3507.99

  311        312        313        314        315        316        317
3016.52    3119.99    3006.85    3159.99    3287.50    3499.99    1089.71

  318        319        320        321        322        323        324
 235.81     481.08       0.00    1624.09       0.00     475.19    3295.99

  325        326        327        328        329        330        331
3377.97    2547.99    3307.55    3247.99    2629.09    3483.99     742.79

  332        333        334        335        336        337        338
 608.74      24.25       0.00    1655.34       0.00     365.43    3119.99

  339        340        341        342        343        344        345
3003.98    2871.99    2922.76    2987.99    2569.60    3375.99     736.78

  346        347        348        349        350        351        352
 356.74     640.85       0.00    1650.29       0.00     311.94    3247.99

  353        354        355        356        357        358        359
2585.78    2395.99    4039.88    3291.99    2696.14    3315.99     611.06

  360        361        362        363        364        365        366
 668.83     152.10      38.49    1383.93      75.91     827.23    3135.99
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   367       368       369       370       371       372       373
 2474.24   2951.99   2199.09   3067.99   2680.22   3415.99    679.77

   374       375       376       377       378       379       380
  845.10      0.00    249.63    804.58    494.84    200.68   2751.99

   381       382       383       384       385       386       387
 2078.61   2727.99   2029.01   2867.99   2684.61   3307.99   1217.03

   388       389       390       391       392       393       394
  472.95    517.19     43.90   1108.75    141.27    303.36   2791.99

   395       396       397       398       399       400       401
 1798.74   2767.99   1666.29   2715.99   2338.26   3267.99   1199.00

   402       403       404       405       406       407       408
  367.15    509.82    388.69    292.06    611.05      0.00   2555.99

   409       410       411       412       413       414       415
 1594.35   2443.99   1532.63   2199.99   1896.67   2739.99   1104.76

   416       417       418       419       420       421       422
  606.05    135.04    250.83    777.62      0.00     79.30   2095.99

   423       424       425       426       427       428       429
 1492.95   2303.99    875.43   2383.99   1118.38   2155.99   1423.27

   430       431       432       433       434       435       436
  367.60    237.82     38.71    667.61      0.00      0.00   1963.99

   437       438       439       440       441       442       443
 1019.36   2055.99    666.53   2163.99    863.05   2013.99    697.43

   444       445       446       447       448       449       450
   87.47      0.00    158.32    278.76    220.37      0.00   1707.99

   451       452       453       454       455       456       457
 1194.29   1627.99   1079.93   1609.99   1016.16   1645.99    763.61

   458       459       460       461       462       463       464
    0.00    170.61     21.37    179.75      0.00      0.00   1821.99

   465       466       467       468       469       470       471
  645.45   1533.99    897.94   1515.99    701.53   1547.99    399.51

   472       473       474       475       476       477       478
  179.56      0.00      0.00    246.34      0.00      0.00   1409.99
 479       480       481       482       483       484       485
 907. 55  1289. 99   587. 60  1561. 99   470. 20  1395. 99   368. 07

 486       487       488       489       490       491       492
 224. 01     0. 00     0. 00     0. 00     0. 00     0. 00  1119. 99

 493       494       495       496       497       498       499
 674. 49  1235. 99   388. 38  1395. 99   541. 10  1199. 99   106. 18

 500       501       502       503       504       505       506
 287. 31     0. 00   174. 84     0. 00     0. 00     0. 00  1027. 99

 507       508       509       510       511       512       513
 540. 22  1079. 99   146. 40  1505. 99   365. 40  1463. 99   183. 61

 514       515       516       517       518       519       520
 190. 21     0. 00   272. 40     0. 00    68. 35     0. 00  1181. 99

 521       522       523       524       525       526       527
 609. 81  1151. 99   233. 39  1183. 99   222. 25  1537. 99     0. 00

 528       529       530       531       532       533       534
  53. 40   107. 98     0. 00     0. 00     0. 00     0. 00  1197. 99

 535       536       537       538       539       540       541
 307. 51  1137. 99   309. 38  1081. 99   133. 13  1473. 99     0. 00

 542       543       544       545       546       547       548
 219. 44     0. 00    89. 22     0. 00   176. 25     0. 00   799. 99

 549       550       551       552       553       554       555
 635. 67  1045. 99   178. 17   863. 99   575. 23  1018. 99   200. 44

 556       557       558       559       560       561       562
 140. 86     0. 00     0. 00     0. 00    55. 03     0. 00   806. 99

 563       564       565       566       567       568       569
 207. 27  1101. 99   200. 46   877. 99   318. 94   821. 99   503. 66

 570       571       572       573       574       575       576
   0. 00     0. 00    22. 29     0. 00   341. 89     0. 00   913. 99

 577       578       579       580       581       582       583
 446. 85   639. 99   381. 82  1023. 99   269. 33   847. 99   378. 77

 584       585       586       587       588       589       590
   0. 00     0. 00     0. 00   105. 60   199. 41     0. 00  1145. 99

 591       592       593       594       595       596       597
  71. 55   675. 99   567. 51   623. 99   595. 62   730. 99   454. 22
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598       599       600       601       602       603       604
  0.00    489.17      0.00    278.22      8.06      0.00    698.99

605       606       607       608       609       610       611
255.77    917.99    408.43    608.99    580.04    635.99    444.52

612       613       614       615       616       617       618
  0.00    123.79      0.00    430.29      0.00      0.00    784.99

619       620       621       622       623       624       625
171.73    663.99    277.33    805.99    113.32    693.99    287.82

626       627       628       629       630       631       632
  0.00      0.00      4.86    186.73     73.48      0.00    537.99

633       634       635       636       637       638       639
348.74    626.99    301.96    630.99    223.38    954.99    134.96

640       641       642       643       644       645       646
  0.00      0.00      0.00    370.53      0.00      0.00    347.99
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SHELLA3SS.MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

                                        SR ARRAY


     143       144       145       146       147       148       149
      0.00      0.00      0.00      0.00  43877.90      0.00      0.00

     150       151       152       153       154       155       156
      0.00      0.00      0.00      0.00      0.00      0.00      0.00

     157       158       159       160       161       162       163
      0.00      0.00      0.00      0.00  29049.40      0.00      0.00

     164       165       166       167       168       169       170
      0.00      0.00      0.00      0.00      0.00      0.00      0.00

     171       172       173       174       175       176       177
      0.00      0.00      0.00      0.00  24186.00      0.00      0.00

     178       179       180       181       182       183       184
      0.00      0.00      0.00      0.00      0.00      0.00      0.00

     185       186       187       188       189       190       191
      0.00      0.00      0.00      0.00  21185.10      0.00      0.00

     192       193       194       195       196       197       198
      0.00      0.00      0.00      0.00      0.00   9413.19      0.00

     199       200       201       202       203       204       205
      0.00      0.00      0.00      0.00  16140.50      0.00      0.00

     206       207       208       209       210       211       212
      0.00      0.00      0.00      0.00      0.00   5963.56      0.00

     213       214       215       216       217       218       219
      0.00      0.00   9288.08      0.00  12424.40      0.00      0.00

     220       221       222       223       224       225       226
      0.00      0.00      0.00      0.00      0.00   3891.10      0.00

     227       228       229       230       231       232       233
      0.00      0.00   7361.37      0.00   9728.08      0.00      0.00

     234       235       236       237       238       239       240
      0.00      0.00      0.00      0.00      0.00   2778.85      0.00

     241       242       243       244       245       246       247
   7184.86      0.00   5928.53      0.00   7732.30      0.00   2613.33
   248        249        250        251        252        253        254
    0.00       0.00       0.00       0.00       0.00    1979.91       0.00

   255        256        257        258        259        260        261
 5673.52       0.00    4843.36       0.00    6228.89       0.00    1065.54

   262        263        264        265        266        267        268
    0.00       0.00       0.00    3264.35       0.00    1438.63       0.00

   269        270        271        272        273        274        275
 4635.52       0.00    4008.02       0.00    4822.71       0.00     398.75

   276        277        278        279        280        281        282
    0.00       0.00       0.00    2331.83       0.00    1114.59       0.00

   283        284        285        286        287        288        289
 4035.29       0.00    3355.53       0.00    3883.76       0.00     773.39

   290        291        292        293        294        295        296
    0.00     106.81       0.00    1740.79       0.00     933.32       0.00

   297        298        299        300        301        302        303
 3340.26       0.00    2839.09       0.00    3345.46       0.00     392.78

   304        305        306        307        308        309        310
    0.00     116.44       0.00    1374.57       0.00     725.58       0.00

   311        312        313        314        315        316        317
 2903.61       0.00    2425.40       0.00    2926.04       0.00     916.73

   318        319        320        321        322        323        324
    0.00     123.51       0.00    1091.22       0.00     475.19       0.00

   325        326        327        328        329        330        331
 2497.25       0.00    2090.37       0.00    2477.72       0.00     742.79

   332        333        334        335        336        337        338
    0.00      24.25       0.00     925.50       0.00     365.43       0.00

   339        340        341        342        343        344        345
 2165.46       0.00    1816.33       0.00    2113.98       0.00     604.04

   346        347        348        349        350        351        352
    0.00     147.86       0.00     790.65       0.00     311.94       0.00

   353        354        355        356        357        358        359
 1892.02       0.00    1590.09       0.00    1816.25       0.00     530.13

   360        361        362        363        364        365        366
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    0. 00      152. 10        0. 00     679. 97        0. 00     377. 60        0. 00

   367         368          369         370          371         372          373
  1664. 74       0. 00     1401. 73       0. 00     1570. 56       0. 00      464. 09

   374         375          376         377          378         379          380
     0. 00       0. 00        0. 00     588. 41        0. 00     200. 68        0. 00

   381         382          383         384          385         386          387
  1474. 30       0. 00     1243. 66       0. 00     1366. 25       0. 00      408. 71

   388         389          390         391          392         393          394
     0. 00       0. 00        0. 00     512. 12        0. 00     303. 36        0. 00

   395         396          397         398          399         400          401
  1313. 58       0. 00     1110. 05       0. 00     1195. 17       0. 00      351. 40

   402         403          404         405          406         407          408
     0. 00       0. 00        0. 00     292. 06        0. 00       0. 00        0. 00

   409         410          411         412          413         414          415
  1176. 99       0. 00      996. 35       0. 00     1050. 98       0. 00      318. 97

   416         417          418         419          420         421          422
     0. 00       0. 00        0. 00     394. 08        0. 00       0. 00        0. 00

   423         424          425         426          427         428          429
  1060. 17       0. 00      875. 43       0. 00      928. 69       0. 00      291. 01

   430         431          432         433          434         435          436
     0. 00       0. 00        0. 00     348. 19        0. 00       0. 00        0. 00

   437         438          439         440          441         442          443
   959. 66       0. 00      666. 53       0. 00      824. 40       0. 00      266. 77

   444         445          446         447          448         449          450
     0. 00       0. 00        0. 00     278. 76        0. 00       0. 00        0. 00

   451         452          453         454          455         456          457
   872. 71       0. 00      742. 42       0. 00      734. 98       0. 00      245. 64

   458         459          460         461          462         463          464
     0. 00       0. 00        0. 00     179. 75        0. 00       0. 00        0. 00

   465         466          467         468          469         470          471
   645. 45       0. 00      679. 14       0. 00      657. 92       0. 00      227. 13

   472         473          474         475          476         477          478
     0. 00       0. 00        0. 00     246. 34        0. 00       0. 00        0. 00
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479            480            481            482            483            484            485
730.98           0.00         587.60           0.00         470.20           0.00         210.83

486            487            488            489            490            491            492
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

493            494            495            496            497            498            499
672.95           0.00         388.38           0.00         533.16           0.00         106.18

500            501            502            503            504            505            506
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

507            508            509            510            511            512            513
540.22           0.00         146.40           0.00         365.40           0.00         183.61

514            515            516            517            518            519            520
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

521            522            523            524            525            526            527
576.44           0.00         233.39           0.00         222.25           0.00           0.00

528            529            530            531            532            533            534
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

535            536            537            538            539            540            541
307.51           0.00         309.38           0.00         133.13           0.00           0.00

542            543            544            545            546            547            548
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

549            550            551            552            553            554            555
500.21           0.00         178.17           0.00         364.35           0.00           0.00

556            557            558            559            560            561            562
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

563            564            565            566            567            568            569
207.27           0.00         200.46           0.00         318.94           0.00           0.00

570            571            572            573            574            575            576
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

577            578            579            580            581            582            583
439.10           0.00         378.36           0.00         269.33           0.00           0.00

584            585            586            587            588            589            590
   0.00           0.00           0.00           0.00           0.00           0.00           0.00

591            592            593            594            595            596            597
```

```
  71.55       0.00     356.35       0.00     282.17       0.00       0.00

 598        599        600        601        602        603        604
    0.00       0.00       0.00       0.00       0.00       0.00       0.00

 605        606        607        608        609        610        611
 255.77       0.00     336.45       0.00     260.43       0.00       0.00

 612        613        614        615        616        617        618
    0.00       0.00       0.00       0.00       0.00       0.00       0.00

 619        620        621        622        623        624        625
 171.73       0.00     277.33       0.00     113.32       0.00       0.00

 626        627        628        629        630        631        632
    0.00       0.00       0.00       0.00       0.00       0.00       0.00

 633        634        635        636        637        638        639
 348.74       0.00     301.96       0.00     223.38       0.00       0.00
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SHELLA3SS.MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

       NPASS    =   1


BA(I)  1620550.0 822482.0 401920.0 440651.0 162888.0 106022.0 101962.0
BB(I)  2753340.01281920.0 693932.0 621615.0 239357.0 169470.0 152271.0

  STERANS DIV           6981.3    3348.0    2852.8


AROMATICS DIV        5911900.0


 2750480.0 1178650.0  685454.0  503895.0  218585.0  154055.0  115095.0
       0.0  103264.0    8477.5  103759.0    7453.8    4489.7       0.0
    2859.9       0.0       0.0   13959.8   13317.8   10925.0   37175.5


SUM S(I):             193241.0
SA(I):               1772740.0 1977280.0 1143590.0  452898.0
BL(I):                  7935.4   11745.2   14120.4   23066.3


SATSAN NPASS    =   1


SA(I)  1668850.01895190.01119280.0 394947.0
SB(I)  2488750.02761520.01940270.01452290.0
```

```
SHELLA3SS. MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

        NPASS    =   2


BA(I)  1433260. 0 783047. 0 395155. 0 448587. 0 174633. 0 120142. 0 125028. 0
BB(I)  2411130. 01236320. 0 685873. 0 642194. 0 261184. 0 194822. 0 193439. 0

  STERANS DIV             6981. 3    3348. 0    2852. 8


AROMATICS DIV          5624970. 0


 2408260. 0 1130130. 0  677305. 0  531477. 0  238518. 0  177101. 0  146212. 0
       0. 0  106192. 0    8568. 2  110717. 0    8133. 5    5161. 3       0. 0
    2866. 9       0. 0       0. 0       0. 0   14532. 3   12559. 4   47226. 4


SATSAN NPASS     =   2


SA(I)  1677260. 01900930. 01121180. 0 399448. 0
SB(I)  2503470. 02769540. 01933980. 01471800. 0
SHELLA3SS. MI  01/24/86
1UL HYDROCARBON STD C5-C40 FOR E

                      MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                1. 01186



SUM OF PEAK HEIGHTS               13114300. 0
SUM OF DE-ISOTOPED PEAKS          11967400. 0

DENSITY OF TEST SAMPLE                    0. 8787

AMOUNT OF RECOVERY                      109. 0


AVERAGE MOLECULAR WEIGHT                199. 9



                                                 *
                                                 *  ESTIMATED
                                    VOLUME PCT   *  WEIGHT PCT
                                   ------------  * -------------
    SATURATES                              57. 1 *          53. 7
       PARAFFINS                   16. 4         * 14. 2
       NONCOND CYCLOPARAFFINS      18. 2         * 16. 7
       COND CYCLOPAR 2-RING        12. 7         * 12. 5
       COND CYCLOPAR 3-RING+        9. 6         * 10. 1
    AROMATICS                              42. 8 *          46. 2
     MONO-                             32. 1     *      32. 7
       BENZENES                    18. 3         * 17. 9
       NAPHTHENEBENZENES            8. 6         *  9. 2
       DINAPHTHENEBENZENES          5. 1         *  5. 5
     DI-                                7. 2     *       8. 5
       NAPHTHALENES                 4. 0         *  4. 6
       ACENAPHTHENES, DBZFURANS     1. 8         *  2. 2
       FLUORENES                    1. 3         *  1. 7
     TRI-                               1. 1     *       1. 5
       PHENANTHRENES                1. 1         *  1. 4
  NAPHTHENEPHENANTHRENES    0.0            *  0.0
TETRA-                          0.8        *        1.2
  PYRENES                   0.8            *  1.1
  CHRYSENES                 0.0            *  0.0
PENTA-                          0.1        *        0.1
  PERYLENES                 0.0            *  0.0
  DIBENZANTHRACENES         0.0            *  0.0
THIOPHENO-                      0.8        *        1.1
  BENZOTHIOPHENES           0.0            *  0.0
  DIBENZOTHIOPHENES         0.8            *  1.1
  NAPHTHOBENZOTHIOPHENES    0.0            *  0.0
UNIDENTIFIED                    0.5        *        0.8
  CLASS I  WITH NAPHPHENAN                 *
  CLASS II                  0.0            *  0.0
  CLASS III                 0.0            *  0.0
  CLASS IV                  0.0            *  0.0
  CLASS V                   0.1            *  0.1
  CLASS VI                  0.0            *  0.1
  CLASS VII                 0.3            *  0.5
```

DATA ACQUISITION
AND
PROCESSING PROCEDURES

```
TRACE OF PROCEDURE EMPS
    * ACQU(01250; S; E)
    * WAIT #55
    * BEEP; BEEP
    * WAIT #60
    * BEEP; BEEP; BEEP
    * ACQU(S; E)
    * MAP/C(D60, 1250; E)
    *
    * BEEP; BEEP
    *
    *
    *
    ACQU  (01250; S; E)
    WAIT #55
    BEEP
    BEEP
    WAIT #60
    BEEP
    BEEP
    BEEP
    ACQU  (S; E)
    MAP  (D60, 1250; E)/C
    BEEP
    BEEP
```

```
TRACE OF PROCEDURE EMR
   * SETN EMR
   * EMR1
   * ERASE
   *
   SETN EMR
   EMR1
      * GETN
      * SET1
      * SET3 $
      * CHRO(I; H; E)
      * ADSA(1; 1250; 0)/BX
      * TOGGLE
      * SPEC(D34, 300, V0; H; E)
      * ROBINS(H; G200; E)
      * LOOP
      *
      GETN
      SET1
      SET3 $
      CHRO  (I; H; E)
      ADSA  (1; 1250; 0)/BX
      TOGGLE
         * SET6 $1
         * SET1 $3
         * SET3 $6
         *
         SET6 $1
         SET1 $3
         SET3 $6
      SPEC  (D34, 300; V0; H; E)
      ROBINS  (H; G200, E)
         * RUN ROBINS
         *
         RUN ROBINS
      LOOP
   ERASE
```

```
TRACE OF PROCEDURE EMR2
    * SETN EMR1
    * EMR3
    * ERASE
    *
    SETN EMR1
    EMR3
        * GETN
        * SET3 $
        * CHRO(I; H; E)
        * ADSA(1, 1750; 0)/BX
        * TOGGLE
        * SPEC(D34, 300; V0; H; E)
        * ROBINS(H; G200; E)
        * LOOP
        *
        GETN
        SET3 $
        CHRO   (I; H; E)
        ADSA   (1, 1750; 0)/BX
        TOGGLE
            * SET6 $1
            * SET1 $3
            * SET3 $6
            *
            SET6 $1
            SET1 $3
            SET3 $6
        SPEC   (D34, 300; V0; H; E)
        ROBINS   (H; G200; E)
            * RUN ROBINS
            *
            RUN ROBINS
        LOOP
    ERASE
```

```
TRACE OF PROCEDURE EMMR
   * SETN EMMR
   * EMRS
   * ERASE
   *
   SETN EMMR
   EMRS
      * GETN
      * SET1
      * SET3 $
      * CHRO(I; H; E)
      * ADSA(1; 800; 0)/BX
      * TOGGLE
      * SPEC(D34, 300; V0; H; E)
      * ROBINS(H; G200; E)
      * LOOP
      *
      GETN
      SET1
      SET3 $
      CHRO   (I; H; E)
      ADSA   (1; 800; 0)/BX
      TOGGLE
         * SET6 $1
         * SET1 $3
         * SET3 $6
         *
         SET6 $1
         SET1 $3
         SET3 $6
      SPEC   (D34, 300; V0; H; E)
      ROBINS   (H; G200; E)
         * RUN ROBINS
         *
         RUN ROBINS
      LOOP
   ERASE
```

APPENDIX B

USERS MANUAL

ROBINSON'S METHOD FOR HYDROCARBON ANALYSIS USER'S MANUAL

Version 1.0 860617

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USER'S MANUAL

1. Introduction

The program characterizes heavy gas oils using a technique developed by C.J. Robinson in the late 1960's (Analytical Chemistry, Vol 43, #11, 1971). The program is fully MSDS compatible and operates with the same command format as the standard MSDS routines. This manual assumes that the user is familiar with the syntax of MSDS commands in general.

2. Data acquisition

The data acquired for analysis by this routine must start below mass 43. If mass 43 is not included in the scan the analysis will not be correct. The highest mass number that will be accepted is 758. Peaks above 758 are ignored.

3. Data reduction

Before the main analysis can be run the data must be transformed into a single scan of data in a mass vs. intensity file. To do this the MSDS routine ADSA (ADD and SAVE) is used. Documentation on this routine is contained in the old MSDS manual (20000-90193 Volume 1).

The routine can be run with the command:

```
>ADSA infile,califile,outfile/BX
```

The three file names can be omitted if they are already in place (main file, cali file, auxiliary file). The "BX" modifier ensures that outfile starts at the beginning (any previous data is lost). The infile is usually a time intensity file (.TI) and ADSA produces a mass intensity file (.MI and .MX Only the .MI file is used). The infile and outfile can be the same name.

4. Running the analysis

To start the analysis type:

```
>ROBINS,filename
```

where filename is a valid mass intensity file. The system will respond with the prompt "ROBINS:". To produce a printed output of the analysis use the commands: ROBINS: **H;Gx;E** where x is the average molecular weight of the sample. The analysis will be performed, the results printed, and the system will return to MSDS.

5. Program commands

ROBINS accepts some of the standard MSDS commands such as "?" which will give a summary of all of the available commands. This summary is reproduced in figure 1. Other standard commands are present and function the way they would in CHRO for example: "**Q**" gives a hardcopy of the command summary; "**@XY**" runs the method ROBIXY; "b" reruns the current method; "E" exits to the MSDS executive;

FIGURE 1: THE HELP PAGE FOR ROBINS

```
ROBINS  ACCEPTS THE FOLLOWING COMMANDS:                         25/07/85

DEBUGGING AIDS

R        READ IN THE DATA
L        LIST THE FULL SPECTRUM TO THE CURRENT OUTPUT DEVICE
T        PRINT ALL INTERMEDIATE RESULTS
A X      RUN THE ANALYSIS WITH AVERAGE MOL WT X

STANDARD COMMANDS

G X      READ DATA AND RUN THE ANALYSIS WITH AVG. MOL. WT. X
S        SET THE PARAMETERS
K        KEEP THE PARAMETERS
I        INITIALIZE THE PARAMETERS
P        READ THE PARAMETERS FROM THE PARAMETER FILE

D        FURTHER OUTPUT TO THE TERMINAL
H (^)    FURTHER OUTPUT TO THE PRINTER (WITH EXTRA FORM FEED)
E        EXIT TO MSDS
ID       EXIT TO IDOS
@CD      RUN METHOD CD
@        LOOP TO BEGINNING OF CURRENT METHOD
Q        HARDCOPY THIS EXPLANATION PAGE
?        PRODUCE THIS EXPLANATION PAGE
```

"ID" exits to IDOS. "H" is the hardcopy command which directs that all *further* output be sent to the printer. This is slightly different from the "H" command used in many of the standard MSDS programs. The complement of "H" is the "D" command which reverts to printing further output on the display terminal.

The command which will normally be used to run the analysis is the "G x" command. "x" is the average molecular weight of the mixture as determined previously by some appropriate method. If "x" is missing a default value of 1.0 is assumed for calculations.The analysis will be performed and a one page summary of results will be printed to the currently selected output device (see "D" and "H" commands).

If it is necessary to have more output than the one page summary results, the user can use the debugging commands. These commands allow you to print out a number of intermediate results. The "R" command reads in the spectrum from the mass intensity file and performs the deisotoping calculations as well. The "L" command lists the full spectrum of poly and monoisotopic peaks to the current output device. This may be useful as a hardcopy record of the data. The "T" command sets a flag which prints a number of important intermediate results from several places in the analysis. These will probably not be useful except to programmers making modifications to the code. The "A x" command starts the analysis with the data previously read in via the "R" command. "R;A x" is equivalent the the "G x" discussed previously.

The four commands to set, keep, read and initialize the parameters operate in the same manner that they would with standard MSDS programs. This program has only one parameter which is called AINF. It is usually about 1. The "I" command initializes this parameter to 1. The "S" command allows you to change the parameter. The "K" command saves the current parameter in the parameter file and the "P" command reads the parameter file for a value (note that if the parameter file does not exist this command is the same as the "I" command).

Figure 2 shows an example session with operator inputs shown in **bold.**

6. Multiple file analysis

The procedure file EMR.PR included with this package is an example of a multiple file analysis procedure. It assumes that the name list file EMR.NL contains the names of a series of time intensity files to be reduced and analyzed. All of the standard procedure file structures can be used with this routine.

7. Caution

We have seen problems with this program which pertain to errors caused by division by zero somewhere in the analysis. Most of the error producing sections of code have been modified to watch for the potential occurrence of errors; however, the problem can still be seen occasionally. If an error occurs, an error message will be printed on the screen (note that if nobody is watching the screen when the errors occur, they can be missed because the system never prints them on the printer). The analysis will also very likely produce unreasonable results.
These problems occur when the program is expecting to see peaks which are not

present in the acquisition. This is often due to a completely aromatic sample.

FIGURE 2: EXAMPLE SESSION

```
> ROBINS  TESTFILE          ( extension is forced to .MI )
( screen is cleared )
ROBINS: R                   ( read in the data )
ROBINS: H                   ( hardcopy further results )
ROBINS: T                   ( type all intermediate results )
ROBINS: A247                ( do analysis with MW of 247 )
( results are printed on the printer as given in appendix )
ROBINS: E                   ( exit to MSDS )
>
```

APPENDIX C

SOFTWARE TEST OUTPUTS

```
OBINS.MS TEST DATA FILE:  ROBINTST.FO.  TYPED 25/07/85 TW.  FROM
AMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.  10X VALUES.

      SUM OF POLY AND MONO PEAKS FOR THIS TABLE:      573273.   529319.

           MASS SPECTRUM:  TOP-POLYISOTOPIC, BOTTOM-MONOISOTOPIC



    17         18         19         20         21         22         23
    0.0        0.0        0.0        0.0        0.0        0.0        0.0
    0.00       0.00       0.00       0.00       0.00       0.00       0.00

    24         25         26         27         28         29         30
   37.9      112.9     1304.9    15201.9     2696.9    19473.9      433.9
   37.99     112.17    1302.55   15173.40    2361.93   19419.50       0.00

    31         32         33         34         35         36         37
    0.0        0.0        0.0        0.0        0.0       20.9      226.9
    0.00       0.00       0.00       0.00       0.00      20.99     226.31

    38         39         40         41         42         43         44
  757.9     9329.0     1509.9    28068.9     5291.0    32901.9     1108.9
  750.61    9304.34    1203.77   28025.80    4360.56   32746.10      10.90

    45         46         47         48         49         50         51
  168.9       16.9       21.9        0.0       67.9     1489.9     3552.9
  156.02      10.24      21.44       0.00      67.98    1487.04    3488.19

    52         53         54         55         56         57         58
 1020.9     3580.9     1972.9    21469.9     8380.0    27968.9     1391.9
  867.52    3540.44    1816.61   21387.20    7431.32   27622.70     154.59

    59         60         61         62         63         64         65
   95.9       30.0      212.9      975.0     3096.9     1514.9     2089.9
   68.07      26.20     211.50     963.50    3044.37    1347.92    2012.69

    66         67         68         69         70         71         72
  673.9     5626.0     2543.9    13120.9     6039.0    14576.9      847.9
  562.07    5592.67    2235.13   12990.60    5316.49   14265.40      46.69

    73         74         75         76         77         78         79
  190.9     1576.9     1799.9     2751.9     4928.0     1770.9     2811.9
  170.42    1565.85    1697.65    2638.33    4752.25    1454.44    2707.78

    80         81         82         83         84         85         86
  988.9     6420.0     4166.0     9616.0     3449.9     8592.0     1043.9
  807.87    6361.69    3743.27    9355.85    2820.75    8386.53     478.36
 1133. 9      910. 9     2423. 9     607. 9     5462. 0     1536. 9     1678. 9
 1086. 18     827. 40    2358. 18    425. 70    5423. 47    1119. 79    1579. 16

   94          95          96         97          98          99         100
  977. 9     5836. 0     3083. 9    7710. 0     2336. 9     1998. 9      371. 9
  853. 51    5766. 08    2635. 93   7490. 89    1748. 67    1843. 48     223. 76

  101         102         103        104         105         106         107
  793. 9     1208. 9     1271. 9    1004. 9     5233. 0     2145. 9     1276. 9
  771. 68    1141. 08    1169. 70    898. 78    5150. 25    1690. 57    1110. 78

  108         109         110        111         112         113         114
  710. 9     3716. 9     1737. 9    4107. 0     1724. 9     1841. 9      530. 0
  607. 34    3659. 58    1412. 27   3969. 28    1367. 89    1706. 63     373. 27

  115         116         117        118         119         120         121
 6186. 0     1532. 9     2246. 9    1099. 9     4683. 0     1962. 9     1053. 9
 6146. 73     927. 16    2129. 18    885. 94    4586. 22    1505. 33     884. 78

  122         123         124        125         126         127         128
  533. 9     2321. 9      995. 0    2036. 9     1659. 9     2768. 9     4989. 0
  439. 58    2274. 41     766. 64   1950. 49    1461. 83    2614. 12    4720. 65

  129         130         131        132         133         134         135
 3077. 9     1170. 9     3911. 9    1131. 9     2693. 9     1248. 9      983. 9
 2592. 78     865. 93    3803. 06    709. 87    2595. 29     959. 48     864. 05

  136         137         138        139         140         141         142
  447. 9     1518. 9      760. 0    2842. 9     1447. 9    10526. 9     6389. 0
  347. 37    1475. 85     594. 76   2768. 92    1137. 45   10385. 10    5227. 18

  143         144         145        146         147         148         149
 2207. 9      906. 9     4170. 0    1337. 9     1507. 9      852. 9     1003. 9
 1567. 43     688. 62    4076. 48    840. 69    1379. 10     680. 27     912. 23

  150         151         152        153         154         155         156
  801. 9     2019. 9     3998. 9    3622. 9     2093. 9     8540. 0     8295. 0
  686. 62    1930. 34    3759. 30   3151. 59    1683. 75    8312. 75    7266. 26

  157         158         159        160         161         162         163
 2029. 9      737. 9     2357. 9    1309. 9     1118. 9      894. 9     1354. 9
 1082. 83     545. 54    2277. 45   1005. 05     967. 96     758. 88    1246. 70

  164         165         166        167         168         169         170
  802. 9     4827. 0     1851. 9    3117. 9     2355. 9     4343. 0     5813. 0
  631. 58    4733. 08    1217. 93   2917. 50    1957. 51    4058. 17    5255. 27

  171         172         173        174         175         176         177
 1441. 9      506. 9     1081. 9     900. 9      787. 9     1284. 9     1068. 9
  706. 41     362. 89    1023. 46    751. 11     670. 70    1181. 68     892. 99

  178         179         180        181         182         183         184
```

```
2478. 40     2460. 95     1183. 88     2490. 70     2441. 20     1580. 34     2533. 88


 185          186          187          188          189          190          191
 775. 9       396. 9       627. 9       640. 9      1633. 9      1059. 9      1999. 9
 393. 91      311. 75      575. 62      548. 79     1542. 91      815. 52     1856. 72


 192          193          194          195          196          197          198
2571. 9      2089. 9      1554. 9      1840. 9      2283. 9      1167. 9      1360. 9
2275. 48     1716. 67     1263. 28     1625. 62     2017. 17      835. 91     1208. 08


 199          200          201          202          203          204          205
 453. 9       397. 9       375. 9       871. 9       642. 9       637. 9      1040. 9
 256. 26      342. 02      316. 24      815. 35      504. 04      544. 07      944. 34


 206          207          208          209          210          211          212
2124. 9      1081. 9      1164. 9       932. 9      1398. 9       766. 9       902. 9
1961. 32      744. 12     1015. 99      754. 34     1260. 22      547. 16      795. 32


 213          214          215          216          217          218          219
 318. 9       224. 9       379. 9       375. 0       350. 0       522. 9       451. 9
 179. 07      183. 07      345. 11      311. 43      289. 95      467. 19      365. 10


 220          221          222          223          224          225          226
 937. 9       478. 9       602. 9       390. 0       706. 9       406. 9       528. 9
 866. 49      320. 09      533. 44      290. 59      647. 48      287. 58      468. 20


 227          228          229          230          231          232          233
 173. 9       159. 9       171. 9       226. 9       206. 9       383. 9       255. 9
  86. 34      136. 84      144. 92      197. 55      167. 51      349. 25      187. 55


 234          235          236          237          238          239          240
 315. 9       221. 9       305. 9       172. 9       357. 9       252. 9       255. 9
 274. 88      167. 10      269. 91      119. 29      330. 95      188. 48      214. 79


 241          242          243          244          245          246          247
  93. 9        96. 9        91. 9       143. 9       121. 9       247. 9       159. 9
  50. 18       83. 41       74. 50      127. 64       95. 23      226. 66      113. 08


 248          249          250          251          252          253          254
 148. 9       127. 9       185. 9        98. 9       208. 9       167. 9       144. 9
 122. 21      101. 50      163. 44       64. 44      193. 03      128. 17      115. 68


 255          256          257          258          259          260          261
  58. 0        63. 9        59. 0        96. 9        71. 9       157. 9        96. 9
  32. 39       55. 01       46. 79       85. 03       52. 96      145. 07       65. 39


 262          263          264          265          266          267          268
 100. 9        83. 0       119. 9        60. 0       134. 9       101. 9        97. 9
  34. 19       63. 90      104. 76       36. 56      125. 07       74. 82       79. 54


 269          270          271          272          273          274          275
  35. 0        41. 9        33. 0        61. 9        43. 9        92. 9        53. 0
```

```
276        277        278        279        280        281        282
 61. 9      50. 0      78. 0      37. 9      82. 0      64. 9      60. 0
 52. 60     37. 55     68. 44     21. 93     75. 52     47. 70     47. 61

283        284        285        286        287        288        289
 22. 9      29. 0      21. 9      39. 9      26. 0      60. 0      36. 0
 11. 28     25. 26     15. 85     35. 67     17. 31     55. 06     22. 75

290        291        292        293        294        295        296
 39. 9      23. 9      51. 0      22. 9      50. 0      35. 0      38. 9
 33. 28     15. 66     46. 49     11. 76     46. 05     23. 94     32. 21

297        298        299        300        301        302        303
 13. 9      15. 9       0. 0      25. 0       0. 0      33. 0      15. 9
  5. 85     13. 73      0. 00     24. 61      0. 00     32. 30      8. 13

304        305        306        307        308        309        310
 22. 9      14. 9      31. 0      13. 9      28. 0      20. 9      19. 9
 20. 10      7. 86     28. 03      6. 87     25. 52     14. 56     15. 70

311        312        313        314        315        316        317
  0. 0       0. 0       0. 0      12. 9       0. 0      19. 9       0. 0
  0. 00      0. 00      0. 00     12. 99      0. 00     19. 59      0. 00

318        319        320        321        322        323        324
 13. 9       0. 0      15. 9       0. 0      14. 9       7. 9       0. 0
 13. 39      0. 00     15. 58      0. 00     14. 51      4. 29      0. 00

325        326        327        328        329        330        331
  0. 0       0. 0       0. 0       9. 9       0. 0       0. 0       0. 0
  0. 00      0. 00      0. 00      9. 99      0. 00      0. 00      0. 00
```

```
ROBINS.MS TEST DATA FILE:  ROBINTST.FO   TYPED 25/07/85 TW.   FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.   10X VALUES.


                             SATURATES SPECTRUM


    31        32        33        34        35        36        37
     0.00      0.00      0.00      0.00      0.00      0.00      0.00

    38        39        40        41        42        43        44
     0.00      0.00      0.00      0.00      0.00  32901.90      0.00

    45        46        47        48        49        50        51
     0.00      0.00      0.00      0.00      0.00      0.00      0.00

    52        53        54        55        56        57        58
     0.00      0.00      0.00  21469.90      0.00  27968.90      0.00

    59        60        61        62        63        64        65
     0.00      0.00      0.00      0.00      0.00      0.00      0.00

    66        67        68        69        70        71        72
     0.00      0.00      0.00  13120.90   5782.19  14476.80      0.00

    73        74        75        76        77        78        79
     0.00      0.00      0.00      0.00      0.00      0.00      0.00

    80        81        82        83        84        85        86
     0.00   6419.99   3561.57   9613.99   3184.39   8591.99      0.00

    87        88        89        90        91        92        93
     0.00      0.00      0.00      0.00      0.00      0.00   1579.16

    94        95        96        97        98        99       100
   977.99   5766.08   2798.39   7709.99   2133.59   1727.62      0.00

   101       102       103       104       105       106       107
     0.00      0.00      0.00      0.00      0.00      0.00   1110.78

   108       109       110       111       112       113       114
   710.99   3447.35   1679.03   4106.99   1626.81   1285.52      0.00

   115       116       117       118       119       120       121
     0.00      0.00      0.00      0.00      0.00      0.00    884.78

   122       123       124       125       126       127       128
   533.99   2106.91    994.99   1950.49   1182.17    928.40      0.00
   0.00         0.00         0.00         0.00         0.00         0.00       864.05

136          137          138          139          140          141          142
447.99      1028.02       612.93       726.59       731.98       683.89         0.00

143          144          145          146          147          148          149
   0.00         0.00         0.00         0.00         0.00         0.00       820.84

150          151          152          153          154          155          156
390.67       937.08       447.49       423.50       528.57       534.76         0.00

157          158          159          160          161          162          163
   0.00         0.00         0.00         0.00         0.00         0.00       671.08

164          165          166          167          168          169          170
285.57       672.34       358.29       302.40       446.55       451.52         0.00

171          172          173          174          175          176          177
   0.00         0.00         0.00         0.00         0.00         0.00       499.56

178          179          180          181          182          183          184
223.[illegible]       407.63       199.44       226.87       398.37       382.26         0.00

185          186          187          188          189          190          191
   0.00         0.00         0.00         0.00         0.00         0.00       420.77

192          193          194          195          196          197          198
182.77       387.63       252.16       191.65       320.76       305.95         0.00

199          200          201          202          203          204          205
   0.00         0.00         0.00         0.00         0.00         0.00       251.66

206          207          208          209          210          211          212
148.36       [illegible]       207.72       113.99       258.16       244.32         0.00

213          214          215          216          217          218          219
   0.00         0.00         0.00         0.00         0.00         0.00       194.48

220          221          222          223          224          225          226
123.56       180.57       173.99        91.74       206.92       193.84         0.00

227          228          229          230          231          232          233
   0.00         0.00         0.00         0.00         0.00         0.00       136.10

234          235          236          237          238          239          240
104.35       158.06       138.92        64.42       164.45       151.96         0.00

241          242          243          244          245          246          247
   0.00         0.00         0.00         0.00         0.00         0.00       101.67
```

```
248         249         250         251         252         253         254
  86.91      101.50      109.58       46.60      128.87      116.84        0.00

255         256         257         258         259         260         261
   0.00        0.00        0.00        0.00        0.00        0.00       65.39

262         263         264         265         266         267         268
  67.55       63.90       84.78       32.87       98.75       74.82        0.00

269         270         271         272         273         274         275
   0.00        0.00        0.00        0.00        0.00        0.00       33.50

276         277         278         279         280         281         282
  51.06       37.55       63.64       21.48       73.04       47.70        0.00

283         284         285         286         287         288         289
   0.00        0.00        0.00        0.00        0.00        0.00       22.75

290         291         292         293         294         295         296
  36.91       15.66       45.46       11.76       50.00       23.94        0.00

297         298         299         300         301         302         303
   0.00        0.00        0.00        0.00        0.00        0.00        8.13

304         305         306         307         308         309         310
  22.99        7.86       29.72        6.87       27.99       14.56        0.00

311         312         313         314         315         316         317
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

318         319         320         321         322         323         324
  13.99     [illegible] 15.99        0.00       14.99        4.29        0.00
```

```
ROBINS.MS TEST DATA FILE:  ROBINTST.FO.  TYPED 25/07/85 TW.  FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.  10X VALUES.

                          AROMATICS SPECTRUM

  31          32          33          34          35          36          37
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  38          39          40          41          42          43          44
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  45          46          47          48          49          50          51
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  52          53          54          55          56          57          58
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  59          60          61          62          63          64          65
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  66          67          68          69          70          71          72
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  73          74          75          76          77          78          79
   0.00        0.00        0.00        0.00        0.00     1770.99        0.00

  80          81          82          83          84          85          86
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

  87          88          89          90          91          92          93
   0.00        0.00        0.00        0.00     5423.47     1536.99        0.00

  94          95          96          97          98          99         100
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

 101         102         103         104         105         106         107
   0.00        0.00        0.00     1004.99     5150.24     2145.99        0.00

 108         109         110         111         112         113         114
   0.00        0.00        0.00        0.00        0.00        0.00        0.00

 115         116         117         118         119         120         121
   0.00        0.00     2129.18     1099.99     4586.22     1962.99        0.00

 122         123         124         125         126         127         128
   0.00        0.00        0.00        0.00        0.00        0.00     4988.99
  129        130        131        132        133        134        135
2592.78    1170.99    [illegible]803.06    1131.99    2595.29    1248.99       0.00

  136        137        138        139        140        141        142
   0.00       0.00       0.00       0.00       0.00    9701.29    6388.99

  143        144        145        146        147        148        149
1567 43     906.99    4076.48    1337.99    1379.10     852.99       0.00

  150        151        152        153        154        155        156
   0.00       0.00       0.00       0.00    1565.42    7777.98    8294.99

  157        158        159        160        161        162        163
1082.83    [illegible]    1277.48    1309 99     967.96     894.99       0.00

  164        165        166        167        168        169        170
   0.00       0.00    1448.30    2615.18    1909.44    3606.64    5812.99

  171        172        173        174        175        176        177
 706.41     50[illegible].99    1023.46     900.99     670.70     809.33       0.00

  178        179        180        181        182        183        184
2394.20    [illegible]    [illegible]    2363.88    2413 62    1198 08    2785.99

  185        186        187        188        189        190        191
 393.91     [illegible]     475.52     640.99     587.37     723.66    1435.94

  192        193        194        195        196        197        198
2389.[illegible]    [illegible]    [illegible]    1443.96    1963.23     529.96    1360.99

  199        200        201        202        203        204        205
 256.25     [illegible]     316.24     871.99     504.04     637.99     692.67

  206        207        208        209        210        211        212
1976.63     [illegible]     757 27     640.35    1140.83     302 84     902.99

  213        214        215        216        217        218        219
 171.30     224.99     345.11     375.00     289.95     522 99     170.62

  220        221        222        223        224        225        226
 814.43     137.53     429 00     208.64     500.07      93.73     528.99

  227        228        229        230        231        232        233
  86.34     159.99     144.92     226.99     167.51     383.99      51.44

  234        235        236        237        238        239        240
 211.64      29.04     167.07      54 87     193.54      36.51     255.99

  241        242        243        244        245        246        247
  50.18      96.99      74.50     143.99      95.23     247.99      11.40
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248       249       250       251       252       253       254
  62.08      0.00     76.41     17.84     80.12     11.32    144.99

255       256       257       258       259       260       261
  32.39     63.99     46.79     96.99     52.96    157.99      0.00

262       263       264       265       266       267       268
  33.44      0.00     35.21      3.69     36.24      0.00     97.99

269       270       271       272       273       274       275
  16.59     11.99     24.52     61.99     31.11     92.99      0.00

276       277       278       279       280       281       282
  10.93      0.00     14.35      0.44      8.95      0.00     59.99

283       284       285       286       287       288       289
  11.28     28.99     15.85     39.99     17.31     59.99      0.00

290       291       292       293       294       295       296
   3.08      0.00      5.53      0.00      0.00      0.00     38.99

297       298       299       300       301       302       303
   5.85     11.79      0.00     25.00      0.00     32.99      0.00

304       305       306       307       308       309       310
   0.00      0.00      1.27      0.00      0.00      0.00     19.99

311       312       313       314       315       316       317
   0.00      0.00      0.00     12.99      0.00     19.99      0.00

318       319       320       321       322       323       324
   0.00      0.00      0.00      0.00      0.00      0.00      0.00

325       326       327       328       329       330       331
   0.00      0.00      0.00      9.99      0.00      0.00      0.00
```

```
OBINS. MS TEST DATA FILE:  ROBINTST. FO   TYPED 25/07/85 TW.   FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.  10X VALUES.

                                  SR ARRAY

  143        144        145        146        147        148        149
     0. 00      0. 00      0. 00      0. 00   1195. 24      0. 00      0. 00

  150        151        152        153        154        155        156
     0. 00      0. 00      0. 00      0. 00      0. 00      0. 00      0. 00

  157        158        159        160        161        162        163
     0. 00      0. 00      0. 00      0. 00    540. 63      0. 00      0. 00

  164        165        166        167        168        169        170
     0. 00      0. 00      0. 00      0. 00      0. 00      0. 00      0. 00

  171        172        173        174        175        176        177
     0. 00      0. 00      0. 00      0. 00    359. 95      0. 00      0. 00

  178        179        180        181        182        183        184
     0. 00      0. 00      0. 00      0. 00      0. 00      0. 00      0. 00

  185        186        187        188        189        190        191
     0. 00      0. 00      0. 00      0. 00    243. 63      0. 00      0. 00

  192        193        194        195        196        197        198
     0. 00      0. 00      0. 00      0. 00      0. 00    529. 96      0. 00

  199        200        201        202        203        204        205
     0. 00      0. 00      0. 00      0. 00    166. 84      0. 00      0. 00

  206        207        208        209        210        211        212
     0. 00      0. 00      0. 00      0. 00      0. 00    255. 13      0. 00

  213        214        215        216        217        218        219
     0. 00      0. 00    179. 26      0. 00    115. 10      0. 00      0. 00

  220        221        222        223        224        225        226
     0. 00      0. 00      0. 00      0. 00      0. 00     93. 73      0. 00

  227        228        229.       230        231        232        233
     0. 00      0. 00    116. 66      0. 00     79. 68      0. 00      0. 00

  234        235        236        237        238        239        240
     0. 00      0. 00      0. 00      0. 00      0. 00     36. 51      0. 00

  241        242        243        244        245        246        247
```

```
248        249        250        251        252        253        254
   0.00       0.00       0.00       0.00       0.00      11.32       0.00

255        256        257        258        259        260        261
  32.39       0.00      46.73       0.00      37.92       0.00       0.00

262        263        264        265        266        267        268
   0.00       0.00       0.00       3.69       0.00       0.00       0.00

269        270        271        272        273        274        275
  16.59       0.00      24.52       0.00      25.83       0.00       0.00

276        277        278        279        280        281        282
   0.00       0.00       0.00       0.00       0.00       0.00       0.00

283        284        285        286        287        288        289
  11.28       0.00      15.85       0.00      17.31       0.00       0.00

290        291        292        293        294        295        296
   0.00       0.00       0.00       0.00       0.00       0.00       0.00

297        298        299        300        301        302        303
   5.85       0.00       0.00       0.00       0.00       0.00       0.00
```

```
OBINS. MS TEST DATA FILE:   ROBINTST FO    TYPED 25/07/85 TW.   FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.   10X VALUES.

       NPASS    =    1


A(I)      36622. 4  24145. 2  11637. 5  53860. 0  17060. 2   9711. 0  10257. 7
BB(I)     61142. 6  41643. 3  18289. 7 104489. 0  27251. 4  16298. 0  17326. 1

 STERANS DIV                   0. 0         0. 0         0. 0


ROMATICS DIV           286440. 0


   55106. 1   40964. 3   18289 7  104260. 0   27249. 1   16298. 0   17221. 1
    5289. 2     679. 0       0. 0      228. 7        2. 2        0. 0      104. 9
     747. 2       0. 0       0. 0        0. 0        0. 0        0. 0        0. 0


UM S(I):                 7172. 2
SA(I):                  90922. 9   70625. 4   31499. 2   11484. 6
L(I):                     112. 9     265. 1     -28. 4     235. 4

SATSAN NPASS    =    1


SA(I)    107074. 0  90211. 6  32701. 0  11244 5
B(I)     203789. 0 145988 0  75650. 8  46471. 1
```

```
ROBINS. MS TEST DATA FILE:   ROBINTST FO.   TYPED 25/07/85 TW.   FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.   10X VALUES.

      NPASS    =    2


A(I)     31846. 5  23077. 1  12089. 1  53972. 8  17325. 3   9682. 5  10493. 2
SB(I)    51928. 8  40156. 3  19651. 3 104539 0  27768. 2  16155. 4  17855. 8

 STERANS DIV                 0. 0        0. 0        0. 0

AROMATICS DIV          278055. 0

  45816. 7   39461. 5   19651. 3  102774. 0   27765. 9   16155. 4   17747. 7
   5355. 4     694. 7       0. 0     225. 4       2. 2       0. 0     108. 1
    756. 6       0. 0       0. 0    1539. 4       0. 0       0. 0       0. 0

ATSAN NPASS    =    2

A(I)    106558. 0  79718. 9  33646. 7  11270. 7
SB(I)   202942. 0 144962 0  75445 1  46581. 4
```

```
 OBINS. MS TEST DATA FILE:  ROBINTST FO.  TYPED 25/07/85 TW.   FROM
SAMPLE TEST DATA FROM AMOCO RESEARCH CENTER - NAPERVILLE.  10X VALUES.

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS


 UM OF PEAK HEIGHTS               573273.0
SUM OF DE-ISOTOPED PEAKS          529319.0

 ENSITY OF TEST SAMPLE                0.8774

AMOUNT OF RECOVERY                  130.4


AVERAGE MOLECULAR WEIGHT              0.9



                                             *
                                             *  ESTIMATED
                                 VOLUME PCT  *  WEIGHT PCT
                                ------------ * ------------
   SATURATES                            51.4 *          44.6
      PARAFFINS                 22.2         * 17.2
      NONCOND CYCLOPARAFFINS    15.9         * 13.7
      COND CYCLOPAR 2-RING       8.2         *  8.2
      COND CYCLOPAR 3-RING+      5.1         *  5.3
   AROMATICS                            48.5 *          55.3
    MCNO-                           18.3     *     19.1
      BENZENES                   7.9         *  7.9
      NAPHTHENEBENZENES          6.8         *  7.5
      DINAPHTHENEBENZENES        3.4         *  3.7
    DI-                             25.5     *     29.9
      NAPHTHALENES              17.9         * 20.4
      ACENAPHTHENES, DBZFURANS   4.8         *  5.9
      FLUORENES                  2.8         *  3.5
    TRI-                             3.2     *      4.3
      PHENANTHRENES              3.0         *  4.1
      NAPHTHENEPHENANTHRENES     0.1         *  0.1
    TETRA-                           0.1     *      0.1
      PYRENES                    0.1         *  0.1
      CHRYSENES                  0.0         *  0.0
    PENTA-                           0.0     *      0.0
      PERYLENES                  0.0         *  0.0
      DIBENZANTHRACENES          0.0         *  0.0
    THIOPHENO-                       0.9     *      1.3
      BENZOTHIOPHENES            0.9         *  1.2
      DIBENZOTHIOPHENES          0.0         *  0.0
      NAPHTHOBENZOTHIOPHENES     0.0         *  0.0
    UNIDENTIFIED                     0.2     *      0.3
      CLASS I  WITH NAPHPHENAN               *
      CLASS II                   0.0         *  0.0
      CLASS III                  0.0         *  0.0
      CLASS IV                   0.2         *  0.3
      CLASS V                    0.0         *  0.0
      CLASS VI                   0.0         *  0.0
      CLASS VII                  0.0         *  0.0
```

```
FILE: BOB      OUTPUT   A   AMOCO RESEARCH CENTER - NAPERVILLE                PAGE 001

              24      3.8      0.0
              25     11.3      0.0
              26    130.5      0.0
              27   1520.2      0.0
              28    269.7      0.0
              29   1947.4      0.0
              30     43.4      0.0
              36      2.1      0.0
              37     22.7      0.0
              38     75.8      3.4
              39    932.9      0.0
              40    151.0     11.2
              41   2806.9      2.7
              42    529.1     19.6
              43   3290.2      1.5
              44    110.9      0.0
              45     16.9      0.0
              46      1.7      0.0
              47      2.2      0.0
              49      6.8      2.6
              50    149.0      2.4
              51    355.3      5.4
              52    102.1      3.4
              53    358.1      0.0
              54    197.3     11.1
              55   2147.0      6.2
              56    838.0     15.7
              57   2796.9     76.9
              58    139.2      5.1
              59      9.6      0.0
              60      3.0      1.3
              61     21.3      2.8
              62     97.5      5.5
              63    309.7     22.4
              64    151.5     30.0
              65    209.0      6.8
              66     67.4      0.0
              67    562.6      5.6
              68    254.4     10.0
              69   1312.1     75.0
              70    603.9     98.4
              71   1457.7     16.9
              72     84.8      5.5
              73     19.1      4.0
              74    157.7      5.0
              75    180.0     34.3
              76    275.2     59.0
              77    492.8     45.7
              78    177.1     14.1
              79    281.2      7.3
              80     98.9      8.8
              81    642.0     41.8
              82    416.6    127.1
              83    961.6     33.3
              84    345.0     21.9
```

mass *

intensity

half mass intensity

Test data used for output

for example [M/e 57 Pos intensity 2796.9
(" = 57 " 76.9]

```
  85     859.2     10.9
  86     104.4      3.6
  87     113.4      7.9
  88      91.1     19.0
  89     242.4     41.2
  90      60.8     20.3
  91     546.2     10.8
  92     153.7      7.7
  93     167.9     16.5
  94      97.8     62.6
  95     583.6     31.5
  96     308.4     21.4
  97     771.0     16.1
  98     233.7      9.9
  99     199.9      5.3
 100      37.2      7.8
 101      79.4     14.7
 102     120.9     14.8
 103     127.2     11.0
 104     100.5     10.4
 105     523.3      9.6
 106     214.6      9.9
 107     127.7     12.3
 108      71.1      9.2
 109     371.7      8.2
 110     173.8      8.7
 111     410.7      6.5
 112     172.5      0.0
 113     184.2      0.0
 114      53.0      0.0
 115     618.6      0.0
 116     153.3      0.0
 117     224.7      8.3
 118     110.0      0.0
 119     468.3      7.7
 120     136.3      0.0
 121     105.4      4.7
 122      53.4      0.0
 123     232.2      0.0
 124      99.5      0.0
 125     203.7      0.0
 126     166.0      0.0
 127     276.9      0.0
 128     498.9      0.0
 129     307.8      0.0
 130     117.1      0.0
 131     391.2      0.0
 132     113.2      0.0
 133     269.4      0.0
 134     124.9      0.0
 135      98.4      5.0
 136      44.8      0.0
 137     151.9      0.0
 138      76.0      0.0
 139     284.3      0.0
 140       144.8      0.0
 141      1052.7      0.0
 142       638.9      0.0
 143       220.8      0.0
 144        90.7      0.0
 145       417.0      0.0
 146       133.8      0.0
 147       150.8      0.0
 148        85.3      0.0
 149       100.4      0.0
 150        80.2      0.0
 151       202.0      0.0
 152       399.9      0.0
 153       362.3      0.0
 154       209.4      0.0
 155       854.0      0.0
 156       829.5      0.0
 157       203.0      0.0
 158        73.8      0.0
 159       235.8      0.0
 160       131.0      0.0
 161       111.9      0.0
 162        89.5      0.0
 163       135.5      0.0
 164        80.3      0.0
 165       482.7      0.0
 166       185.2      0.0
 167       311.8      0.0
 168       235.6      0.0
 169       434.3      0.0
 170       581.3      0.0
 171       144.2      0.0
 172        50.7      0.0
 173       108.2      0.0
 174        90.1      0.0
 175        78.8      0.0
 176       128.5      0.0
 177       106.9      0.0
 178       261.8      0.0
 179       282.6      0.0
 180       156.2      0.0
 181       268.5      0.0
 182       281.2      0.0
 183       195.7      0.0
 184       278.6      0.0
 185        77.6      0.0
 186        39.7      0.0
 187        62.8      0.0
 188        64.1      0.0
 189       163.4      0.0
 190       106.0      0.0
 191       200.0      0.0
 192       257.2      0.0
 193       209.0      0.0
 194       155.5      0.0
```

```
      195     184.1     0.0
      196     228.4     0.0
      197     116.8     0.0
      198     136.1     0.0
      199      45.4     0.0
      200      39.8     0.0
      201      37.6     0.0
      202      87.2     0.0
      203      64.3     0.0
      204      63.8     0.0
      205     104.1     0.0
      206     212.5     0.0
      207     108.2     0.0
      208     116.5     0.0
      209      93.3     0.0
      210     139.9     0.0
      211      76.7     0.0
      212      90.3     0.0
      213      31.9     0.0
      214      22.5     0.0
      215      38.0     0.0
      216      37.5     0.0
      217      35.0     0.0
      218      52.3     0.0
      219      45.2     0.0
      220      93.8     0.0
      221      47.9     0.0
      222      60.3     0.0
      223      39.0     0.0
      224      70.7     0.0
      225      40.7     0.0
      226      52.9     0.0
      227      17.4     0.0
      228      16.0     0.0
      229      17.2     0.0
      230      22.7     0.0
      231      20.7     0.0
      232      38.4     0.0
      233      25.6     0.0
      234      31.6     0.0
      235      22.2     0.0
      236      30.6     0.0
      237      17.3     0.0
      238      35.8     0.0
      239      25.3     0.0
      240      25.6     0.0
      241       9.4     0.0
      242       9.7     0.0
      243       9.2     0.0
      244      14.4     0.0
      245      12.2     0.0
      246      24.8     0.0
      247      16.0     0.0
      248      14.9     0.0
      249      12.8     0.0
```

```
250    18.6    0.0
251     9.9    0.0
252    20.9    0.0
253    16.8    0.0
254    14.5    0.0
255     5.8    0.0
256     6.4    0.0
257     5.9    0.0
258     9.7    0.0
259     7.2    0.0
260    15.8    0.0
261     9.7    0.0
262    10.1    0.0
263     8.3    0.0
264    12.0    0.0
265     6.0    0.0
266    13.5    0.0
267    10.2    0.0
268     9.8    0.0
269     3.5    0.0
270     4.2    0.0
271     3.3    0.0
272     6.2    0.0
273     4.4    0.0
274     9.3    0.0
275     5.3    0.0
276     6.2    0.0
277     5.0    0.0
278     7.8    0.0
279     3.8    0.0
280     8.2    0.0
281     6.5    0.0
282     6.0    0.0
283     2.3    0.0
284     2.9    0.0
285     2.2    0.0
286     4.0    0.0
287     2.6    0.0
288     6.0    0.0
289     3.6    0.0
290     4.0    0.0
291     2.4    0.0
292     5.1    0.0
293     2.3    0.0
294     5.0    0.0
295     3.5    0.0
296     3.9    0.0
297     1.4    0.0
298     1.6    0.0
300     2.5    0.0
302     3.3    0.0
303     1.6    0.0
304     2.3    0.0
305     1.5    0.0
306     3.1    0.0
```

```
◦FILE: BOB      OUTPUT   A   AMOCO RESEARCH CENTER - NAPERVILLE                                   PAGE 006
                                307         1.4         0.0
                                308         2.8         0.0
                                309         2.1         0.0
                                310         2.0         0.0
                                314         1.3         0.0
                                316         2.0         0.0
                                318         1.4         0.0
                                320         1.6         0.0
                                322         1.5         0.0
                                323         0.8         0.0
                                328         1.0         0.0
                              99999         0.0         0.0
0                                                   MASS SPECTRUM   TOP-POLYISOTOPIC, BOTTOM-MONOISOTOPIC
0
                                              SUM OF POLY, MONO ,AND HALF PEAKS FOR THIS TABLE     57327.     52932.     1283.
                                                                                                   57327.     52932.     1283.

                                                                            mass #
                                                                              intensity
                                                                                  monoisotopic peak intensity
                                                                          24        25        26        27        28        29        30
                                                                           4.        11.       131.      1520.     270.      1947.     43.
                                                                               3.80     11.22    130.26   1517.34    236.19   1941.96       0.0
0
                                                      36        37        38        39        40        41        42        43        44
                                                       2.        23.       76.       933.      151.      2807.     529.      3290.     111.
                                                           2.10     22.63     75.06    930.43    120.38   2802.58    436.06   3274.61       1.0
0
    45        46        47                  49        50        51        52        53        54        55        56        57        58
     17.       2.        2.                  7.        149.      355.      102.      358.      197.      2147.     838.      2797.     139.
        15.60      1.02      2.14                6.80    148.70    348.82     86.75    354.04    181.66   2138.72    743.13   2762.27      15.4
0
    59        60        61        62        63        64        65        66        67        68        69        70        71        72
     10.       3.        21.       98.       310.      152.      209.      67.       563.      254.      1312.     604.      1458.     85.
         6.81      2.62     21.15     96.35    304.44    134.79    201.27     56.21    559.27    223.51   1299.06    531.65   1426.55      4.67
0
    73        74        75        76        77        78        79        80        81        82        83        84        85        86
     19.       158.      180.      275.      493.      177.      281.      99.       642.      417.      962.      345.      859.      104.
        17.04    156.59    169.77    263.83    475.23    145.44    270.78     80.79    636.17    374.33    935.59    282.08    838.65     47.84
0
    87        88        89        90        91        92        93        94        95        96        97        98        99        100
     113.      91.       242.      61.       546.      154.      168.      98.       584.      308.      771.      234.      200.      37.
       108.62     82.74    235.82     42.57    542.35    111.98    157.92     85.35    576.61    263.59    749.09    174.87    184.35      22.3
0
    101       102       103       104       105       106       107       108       109       110       111       112       113       114
     79.       121.      127.      101.      523.      215.      128.      71.       372.      174.      411.      173.      184.      53.
        77.17    114.11    116.97     89.88    515.03    169.06    111.08     60.73    365.96    141.23    396.93    136.79    170.66      37.3
```

```
FILE: BOB      OUTPUT   A   AMOCO RESEARCH CENTER - NAPERVILLE                          PAGE 007

0
   115       116       117       118       119       120       121       122       123       124       125       126       127       128
     619.      153.      225.      110.      468.      196.      105.       53.      232.      100.      204.      166.      277.      499.
0    614.67     92.72    212.92     88.59    458.62    150.53     88.48     43.96    227.44     76.66    195.05    146.18    261.41    472.07

   129       130       131       132       133       134       135       136       137       138       139       140       141       142
     308.      117.      391.      113.      269.      125.       98.       45.      152.       76.      284.      145.     1053.      639.
0    259.28     86.59    380.31     70.99    259.53     95.95     86.41     34.74    147.59     59.48    276.89    113.75   1038.52    522.72

   143       144       145       146       147       148       149       150       151       152       153       154       155       156
     221.       91.      417.      134.      151.       85.      100.       80.      202.      400.      362.      209.      854.      830.
0    156.74     68.86    407.65     84.07    137.91     68.03     91.22     68.66    193.03    375.93    315.16    168.38    831.28    726.63

   157       158       159       160       161       162       163       164       165       166       167       168       169       170
     203.       74.      236.      131.      112.       90.      136.       80.      483.      185.      312.      236.      434.      581.
0    108.28     54.55    227.75    100.51     96.80     75.89    124.67     63.16    473.31    121.79    291.75    195.75    405.82    525.53

   171       172       173       174       175       176       177       178       179       180       181       182       183       184
     144.       51.      108.       90.       79.      129.      107.      262.      283.      156.      269.      281.      196.      279.
0     70.64     36.29    102.35     75.11     67.07    118.17     89.30    247.84    246.10    118.39    249.07    244.12    158.03    253.39

   185       186       187       188       189       190       191       192       193       194       195       196       197       198
      78.       40.       63.       64.      163.      106.      200.      257.      209.      156.      184.      228.      117.      136.
0     39.39     31.18     57.56     54.88    154.29     81.55    185.67    227.55    171.67    126.33    162.56    201.72     83.59    120.81

   199       200       201       202       203       204       205       206       207       208       209       210       211       212
      45.       40.       38.       87.       64.       64.      104.      213.      108.      117.       93.      140.       77.       90.
0     25.63     34.20     31.62     81.54     50.40     54.41     94.43    196.13     74.41    101.60     75.43    126.02     54.72     79.53

   213       214       215       216       217       218       219       220       221       222       223       224       225       226
      32.       23.       38.       38.       35.       52.       45.       94.       48.       60.       39.       71.       41.       53.
0     17.91     18.31     34.51     31.14     29.00     46.72     36.51     86.65     32.01     53.34     29.06     64.75     28.76     46.82

   227       228       229       230       231       232       233       234       235       236       237       238       239       240
      17.       16.       17.       23.       21.       38.       26.       32.       22.       31.       17.       36.       25.       26.
0      8.63     13.68     14.49     19.76     16.75     34.93     18.76     27.49     16.71     26.99     11.93     33.10     18.85     21.46

   241       242       243       244       245       246       247       248       249       250       251       252       253       254
       9.       10.        9.       14.       12.       25.       16.       15.       13.       19.       10.       21.       17.       15.
0      5.02      8.34      7.45     12.76      9.52     22.67     11.31     12.22     10.15     16.34      6.44     19.30     12.82     11.57

   255       256       257       258       259       260       261       262       263       264       265       266       267       268
       6.        6.        6.       10.        7.       16.       10.       10.        8.       12.        6.       14.       10.       10.
       3.24      5.50      4.68      8.60      5.30     14.51      6.54      8.42      6.39     10.48      3.66     12.51      7.48      7.95
```

```
0
    269       270       271       272       273       274       275       276       277       278       279       280       281       282
      4.        4.        3.        6.        4.        9.        5.        6.        5.        8.        4.        8.        7.        6.
     1.66      3.66      2.45      5.57      3.11      8.48      3.35      5.26      3.76      6.84      2.19      7.55      4.77      4.76
0
    283       284       285       286       287       288       289       290       291       292       293       294       295       296
      2.        3.        2.        4.        3.        6.        4.        4.        2.        5.        2.        5.        4.        4.
     1.13      2.53      1.59      3.57      1.73      5.51      2.28      3.33      1.57      4.65      1.18      4.61      2.39      3.22
0
    297       298                 300                 302       303       304       305       306       307       308       309       310
      1.        2.                  3.                  3.        2.        2.        2.        3.        1.        3.        2.        2.
     0.59      1.37                2.46                3.23      0.81      2.01      0.99      2.80      0.69      2.55      1.46      1.57
0
                                  314                 316                 318                 320                 322       323
                                    1.                  2.                  1.                  2.                  2.        1.
                                   1.30                1.96                1.34                1.56                1.45      0.43
0
                                  328
                                    1.
                                   1.00
0
1            MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
0     TEST DATA SET USING MS RUN 1770908
               57327.         52932.        0.8775  130.5
0         AVERAGE MOLECULAR WEIGHT
                                                     *
                                      VOLUME PCT     *  ESTIMATED
                                                     *  WEIGHT PCT
                                     ------------    *  ------------
   SATURATES                                 51.5    *             44.6
      PARAFFINS                      22.2            *  17.2
      NONCOND CYCLOPARAFFINS         15.9            *  13.7
      COND CYCLOPAR 2-RING            8.3            *   8.3
      COND CYCLOPAR 3-RING+           5.1            *   5.3
   AROMATICS                                 48.5    *             55.4
    MONO-                                18.3        *        19.2
      BENZENES                        8.0            *   7.9
      NAPHTHENEBENZENES               6.9            *   7.5
      DINAPHTHENEBENZENES             3.4            *   3.7
    DI-                                  25.6        *        30.0
      NAPHTHALENES                   17.9            *  20.4
      ACENAPHTHENES,DBZFURANS         4.8            *   6.0
      FLUORENES                       2.8            *   3.6
    TRI-                                  3.2        *         4.4
      PHENANTHRENES                   3.1            *   4.2
      NAPHTHENEPHENANTHRENES          0.1            *   0.2
    TETRA-                                0.1        *         0.2
      PYRENES                         0.1            *   0.2
      CHRYSENES                       0.0            *   0.0
```

①

lower plotted digits are MW.

← statistical analysis of sample data

```
    PENTA-                             0.0     *        0.0
      PERYLENES                   0.0          *   0.0
      DIBENZANIHRACENES           0.0          *   0.0
    THIOPHENO-                         1.0     *        1.3
      BENZOTHIOPHENES             0.9          *   1.2
      DIRENZOTHIOPHENES           0.0          *   0.1
      NAPHTHOBENZOTHIOPHENES      0.0          *   0.0
    UNIDENTIFIED                       0.3     *        0.4
      CLASS 1  WITH NAPHPHENAN                 *
      CLASS II                    0.0          *   0.0
      CLASS III                   0.0          *   0.0
      CLASS IV                    0.3          *   0.4
      CLASS V                     0.0          *   0.0
      CLASS VI                    0.0          *   0.0
      CLASS VII                   0.0          *   0.0
0                                         DATE CALCULATED:  JUN  4,1985
```

APPENDIX D

ANALYTICAL DATA

```
CMR1A0337 III  06/27/86
IOL SMR TEST SAMPLE #1

                          MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.69999



SUM OF PEAK HEIGHTS                 6922470.0
SUM OF DE-ISOTOPED PEAKS            6293200.0

DENSITY OF TEST SAMPLE                   0.8915

AMOUNT OF RECOVERY                     100.8


AVERAGE MOLECULAR WEIGHT               199.9



                                                *
                                                *  ESTIMATED
                                  VOLUME PCT    *  WEIGHT PCT
                                 ------------   *  ------------
 SATURATES                                61.0  *            56.4
   PARAFFINS                     19.9           *  16.9
   NONCOND CYCLOPARAFFINS        17.8           *  16.1
   COND CYCLOPAR 2-RING          12.7           *  13.6
   COND CYCLOPAR 3-RING+          7.3           *   9.6
 AROMATICS                                38.7  *            43.5
  MONO-                              22.4       *       23.0
   BENZENES                       6.9           *   6.6
   NAPHTHENEBENZENES              [illegible]   *   8.9
   DINAPHTHENEBENZENES            7.0           *   7.4
  DI-                                 1.1       *       13.3
   NAPHTHALENES                   [illegible]   *   3.3
   ACENAPHTHENES DIBENZOFURANS    4.[illegible] *   5.3
   FLUORENES                      3.7           *   4.6
  TRI-                                2.5       *        3.4
   PHENANTHRENES                  1.8           *   2.5
   NAPHTHENEPHENANTHRENES         0.6           *   0.8
  TETRA-                              0.5       *        0.7
   PYRENES                        0.4           *   0.6
   CHRYSENES                      0.0           *   0.1
  PENTA-                              0.0       *        0.0
   PERYLENES                      0.0           *   0.0
   DIBENZANTHRACENES              0.0           *   0.0
  THIOPHENO-                          2.2       *        2.8
   BENZOTHIOPHENES                1.4           *   1.8
   DIBENZOTHIOPHENES              0.6           *   0.9
   NAPHTHOBENZOTHIOPHENES         0.0           *   0.1
 UNIDENTIFIED                         0.0       *        0.0
   CLASS I  WITH NAPHPHENAN                     *
   CLASS II                       0.0           *   0.0
   CLASS III                      0.0           *   0.0
   CLASS IV                       0.0           *   0.0
   CLASS V                        0.0           *   0.0
   CLASS VI                       0.0           *   0.0
   CLASS VII                      0.0           *   0.0
```

```
EMR180627 MI  06/27/86
1UL EMR TEST SAMPLE #1

                       MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.69996


SUM OF PEAK HEIGHTS                 5739070.0
SUM OF DE-ISOTOPED PEAKS            5220850.0

DENSITY OF TEST SAMPLE                     0.8895

AMOUNT OF RECOVERY                       102.9

AVERAGE MOLECULAR WEIGHT                 199.9


                                                  *
                                                  *  ESTIMATED
                                    VOLUME PCT    *  WEIGHT PCT
                                   -------------  *  -------------
   SATURATES                                61.8  *          57.2
      PARAFFINS                    19.6           * 16.7
      NONCOND CYCLOPARAFFINS       19.2           * 17.5
      COND CYCLOPAR 2-RING         13.1           * 12.8
      COND CYCLOPAR 3-RING+         9.8           * 10.1
   AROMATICS                                38.1  *          42.7
    MONO-                              22.2       *     22.9
      BENZENES                      6.7           *  6.4
      NAPHTHENEBENZENES             8.5           *  9.0
      DINAPHTHENEBENZENES           7.0           *  7.4
    DI-                                10.6       *     12.8
      NAPHTHALENES                  2.9           *  3.3
      ACENAPHTHENES, DIBFURANS      4.1           *  5.0
      FLUORENES                     3.5           *  4.4
    TRI-                                2.4       *      3.2
      PHENANTHRENES                 1.7           *  2.3
      NAPHTHENEPHENANTHRENES        0.6           *  0.9
    TETRA-                              0.5       *      0.7
      PYRENES                       0.4           *  0.6
      CHRYSENES                     0.0           *  0.1
    PENTA-                              0.0       *      0.0
      PERYLENES                     0.0           *  0.0
      DIBENZANTHRACENES             0.0           *  0.0
    THIOPHENO-                          2.2       *      2.9
      BENZOTHIOPHENES               1.6           *  2.0
      DIBENZOTHIOPHENES             0.6           *  0.8
      NAPHTHOBENZOTHIOPHENES        0.0           *  0.0
    UNIDENTIFIED                        0.0       *      0.0
      CLASS I  WITH NAPHPHENAN                    *
      CLASS II                      0.0           *  0.0
      CLASS III                     0.0           *  0.0
      CLASS IV                      0.0           *  0.0
      CLASS V                       0.0           *  0.0
      CLASS VI                      0.0           *  0.0
      CLASS VII                     0.0           *  0.0
```

```
EMR1C0637.MI   [illegible] 07/86
1UL EMR TEST SAMPLE #1

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                0.59996


SUM OF PEAK HEIGHTS                 6260240.0
SUM OF DE-ISOTOPED PEAKS            5688030.0

DENSITY OF TEST SAMPLE                0.8914

AMOUNT OF RECOVERY                   [illegible]

AVERAGE MOLECULAR WEIGHT             [illegible]


                                                *
                                                   ESTIMATED
                                       VOLUME PCT  *  WEIGHT PCT
                                       ----------    -----------
                                             [illegible]  *         57.0
 SATURATES
   PARAFFINS                                        * 15.9
   NONCOND CYCLOPARAFFINS                           * 17.5
   COND CYCLOPAR 2 RING                 [illegible] * 12.7
   COND CYCLOPAR 3 RING+               1[illegible].4 * 10.7
                                             39.4 *         42.9
 AROMATICS
  MONO-                                   22.2    *      22.8
   BENZENES                            6.7        *  6.4
   NAPHTHENEBENZENES                   8.4        *  8.9
   DINAPHTHENEBENZENES                 7.0        *  7.4
                                          10.8    *      13.0
  DI-
   NAPHTHALENES                        2.9        *  3.2
   ACENAPHTHENES, DBIFURANS            4.2        *  5.1
   FLUORENES                           [illegible] *  4.5
                                           2.4    *       3.2
  TRI-
   PHENANTHRENES                       1.7        *  2.3
   NAPHTHENEPHENANTHRENES              0.5        *  0.7
                                           0.5    *       0.7
  TETRA-
   PYRENES                             0.4        *  0.5
   CHRYSENES                           0.0        *  0.0
                                           0.0    *       0.0
  PENTA-
   PERYLENES                           0.0        *  0.0
   DIBENZANTHRACENES                   0.0        *  0.0
                                           [illegible] *       2.9
  THIOPHENO-
   BENZOTHIOPHENES                     1.5        *  1.9
   DIBENZOTHIOPHENES                   [illegible] *  0.9
   NAPHTHOBENZOTHIOPHENES              0.0        *  0.0
                                           0.0    *       0.0
  UNIDENTIFIED
   CLASS I  WITH NAPHTHENAN                       *
   CLASS II                            0.0        *  0.0
   CLASS III                           0.0        *  0.0
   CLASS IV                            0.0        *  0.0
   CLASS V                             0.0        *  0.0
   CLASS VI                            0.0        *  0.0
   CLASS VII                           0.0        *  0.0
```

```
EMR2A0701.MI  07/01/86
1UL EMR TEST SAMPLE #2

                      MASS SPECTRAL ANALYSIS [illegible]
AIN FACTOR                                 0.69996


SUM OF PEAK HEIGHTS                17191700.0
SUM OF DE-ISOTOPED PEAKS           157[illegible]700.0

DENSITY OF TEST SAMPLE                   0.8844

AMOUNT OF RECOVERY                     103.3


AVERAGE MOLECULAR WEIGHT               [illegible]9.9


                                              *
                                              *  ESTIMATED
                                 VOLUME PCT   *  WEIGHT PCT
                                 ------------ *  ------------
  SATURATES                             58.0  *          53.9
     PARAFFINS                   18.0         *  15.4
     NONCOND CYCLOPARAFFINS      19.7         *  18.1
     COND CYCLOPAR 2-RING        12.6         *  12.4
     COND CYCLOPAR 3-RING+        7.6         *  [illegible]
  AROMATICS                             [illegible]  *          46.0
   MONO-                                      *
     BENZENES                    [illegible]         *  [illegible].4
     NAPHTHENEBENZENES           1[illegible].7         *  11.4
     DINAPHTHENEBENZENES         [illegible]         *  [illegible].9
   DI-                                  [illegible]  *      12.[illegible]
     NAPHTHALENES                [illegible]         *  [illegible]
     ACENAPHTHENES, DBZFURANS    [illegible]         *  [illegible]
     FLUORENES                   [illegible]         *  [illegible]
   TRI-                                 [illegible]  *
     PHENANTHRENES               [illegible]         *  [illegible]
     NAPHTHENEPHENANTHRENES      [illegible]         *  [illegible]
   TETRA-                               [illegible]  *
     PYRENES                     [illegible]         *  [illegible]
     CHRYSENES                    0.0         *  [illegible]
   PENTA-                                     *
     PERYLENES                    0.0         *  [illegible]
     DIBENZANTHRACENES            0.0         *  [illegible]
   THIOPHENO-                           [illegible]  *
     BENZOTHIOPHENES              1.3         *  [illegible]
     DIBENZOTHIOPHENES            0.1         *  [illegible]
     NAPHTHOBENZOTHIOPHENES       0.0         *  [illegible]
   UNIDENTIFIED                         [illegible]  *          [illegible]
     CLASS I  WITH NAPHPHENAN                 *
     CLASS II                     0.0         *  [illegible]
     CLASS III                    [illegible]         *  [illegible]
     CLASS IV                     [illegible]         *  [illegible]
     CLASS V                      [illegible]         *  [illegible]
     CLASS VI                     [illegible]         *   0.0
     CLASS VII                    [illegible]         *   0.0
```

```
EMPROCAUL MI [illegible]
1UL EMS TEST SAMPLE [illegible]

                            [illegible] SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                       0.69996


SUM OF PEAK HEIGHTS                   13274600.0
SUM OF DE-ISOTOPED PEAKS            . 16683700.0

DENSITY OF TEST SAMPLE                      0.8857

AMOUNT OF RECOVERY                     102.0


AVERAGE MOLECULAR WEIGHT               197.9


                                                  *
                                                  *  ESTIMATED
                                       VOLUME PCT *  WEIGHT PCT
                                     ------------ * ------------
   SATURATES                                57.9 *         53.8
      PARAFFINS                    1[illegible]    * 14.8
      NONCOND CYCLOPARAFFINS       1[illegible]    * 17.8
      COND CYCLOPAR 2-RING         13.2    * 13.0
      COND CYCLOPAR 3-RING+         [illegible]7    *  9.0
   AROMATICS                                42.0 *         46.1
    MONO-                              27.9      *      28.8
      BENZENES                      [illegible]1    *  9.2
      NAPHTHENEBENZENES            10.7    * 11.4
      DINAPHTHENEBENZENES           7.5    *  [illegible]1
    DI-                                13.9      *      13.1
      NAPHTHALENES                  [illegible]    *  [illegible]
      ACENAPHTHENES/DIBENZOFURANS   4.4    *  [illegible]4
      FLUORENES                     [illegible]0    *  [illegible]
    TRI-                                1.1      *       1.5
      PHENANTHRENES                 0.9    *  1.2
      NAPHTHENEPHENANTHRENES        0.1    *  0.2
    TETRA-                              0.4      *       0.5
      PYRENES                       0.3    *  0.5
      CHRYSENES                     0.0    *  0.0
    PENTA-                              0.0      *       0.0
      PERYLENES                     0.0    *  0.0
      DIBENZANTHRACENES             0.0    *  0.0
    THIOPHENO-                          1.5      *       1.9
      BENZOTHIOPHENES               [illegible]    *  1.7
      DIBENZOTHIOPHENES             0.[illegible]    *  0.1
      NAPHTHOBENZOTHIOPHENES        0.0    *  0.0
   UNIDENTIFIED                         0.0      *       0.0
      CLASS I  WITH [illegible]             *
      CLASS II                      0.0    *  0.0
      CLASS III                     0.0    *  0.0
      CLASS IV                      0.0    *  0.0
      CLASS V                       0.0    *  0.0
      CLASS VI                      0.0    *  0.0
      CLASS VII                     0.0    *  0.0
```

```
EMR200701.MI  07 11/86
1UL EMR TEST SAMPLE #2

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.69996


SUM OF PEAK HEIGHTS               18429700.0
SUM OF DE-ISOTOPED PEAKS          16852900.0

DENSITY OF TEST SAMPLE                0.8864

AMOUNT OF RECOVERY                  100.5


AVERAGE MOLECULAR WEIGHT            199.9



                                                *
                                                *  ESTIMATED
                                    VOLUME PCT  *  WEIGHT PCT
                                   ------------ * ------------
  SATURATES                               57.9  *         53.7
     PARAFFINS                     17.4         * 14.9
     NONCOND CYCLOPARAFFINS        19.7         * 18.0
     COND CYCLOPAR 2-RING          13.1         * 12.8
     COND CYCLOPAR 3-RING+          7.6         *  7.8
  AROMATICS                               42.0  *         46.2
   MONO-                              27.7      *     28.5
     BENZENES                       9.3         *  9.1
     NAPHTHENEBENZENES             10.6         * 11.3
     DINAPHTHENEBENZENES            7.6         *  8.1
   DI-                                10.7      *     12.9
     NAPHTHALENES                   3.2         *  3.6
     ACENAPHTHENES, DBZFURANS       4.4         *  5.4
     FLUORENES                      3.1         *  3.9
   TRI-                                1.1      *      1.4
     PHENANTHRENES                  0.9         *  1.2
     NAPHTHENEPHENANTHRENES         0.1         *  0.2
   TETRA-                              0.4      *      0.6
     PYRENES                        0.4         *  0.5
     CHRYSENES                      0.0         *  0.0
   PENTA-                              0.0      *      0.0
     PERYLENES                      0.0         *  0.0
     DIBENZANTHRACENES              0.0         *  0.0
   THIOPHENO-                          1.9      *      2.5
     BENZOTHIOPHENES                1.5         *  1.9
     DIBENZOTHIOPHENES              0.3         *  0.4
     NAPHTHOBENZOTHIOPHENES         0.0         *  0.0
   UNIDENTIFIED                        0.0      *      0.0
     CLASS I  WITH NAPHPHENAN                   *
     CLASS II                       0.0         *  0.0
     CLASS III                      0.0         *  0.0
     CLASS IV                       0.0         *  0.0
     CLASS V                        0.0         *  0.0
     CLASS VI                       0.0         *  0.0
     CLASS VII                      0.0         *  0.0
```

```
EMP3A0701.MI  07/01/86
1UL  EMR TEST SAMPLE #3

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                0.69996


SUM OF PEAK HEIGHTS              44278200.0
SUM OF DE-ISOTOPED PEAKS         39578400.0

DENSITY OF TEST SAMPLE              0.9416

AMOUNT OF RECOVERY                 89.8


AVERAGE MOLECULAR WEIGHT          199.9



                                                   *
                                                   *  ESTIMATED
                                        VOLUME PCT *  WEIGHT PCT
                                        ---------- * -----------
  SATURATES                                  49.9  *         43.4
     PARAFFINS                         17.5        * 14.1
     NONCOND CYCLOPARAFFINS            15.7        * 14.5
     COND CYCLOPAR 2-RING               5.7        *  6.1
     COND CYCLOPAR 3-RING+         [illegible]     *  8.7
  AROMATICS                                  50.1  *         56.5
   MONO-                                14.3       *       14.3
     BENZENES                      [illegible]     *  4.5
     NAPHTHENEBENZENES                  5.2        *  5.2
     DINAPHTHENEBENZENES                4.1        *  4.4
   DI-                                  17.7       *       22.4
     NAPHTHALENES                  [illegible]     *  6.0
     ACENAPHTHENES/DIBENZOFURANS        7.2        *  5.3
     FLUORENES                          6.8        *  8.9
   TRI-                                  8.3       *       10.5
     PHENANTHRENES                      7.1        *  8.9
     NAPHTHENOPHENANTHRENES             1.2        *  1.5
   TETRA-                                1.2       *        1.6
     PYRENES                            0.9        *  1.2
     CHRYSENES                          0.3        *  0.4
   PENTA-                                0.0       *        0.0
     PERYLENES                          0.0        *  0.0
     DIBENZANTHRACENES                  0.0        *  0.0
   THIOPHENO-                            5.7       *        7.4
     BENZOTHIOPHENES                    1.4        *  1.7
     DIBENZOTHIOPHENES                  4.0        *  5.2
     NAPHTHOBENZOTHIOPHENES             0.3        *  0.4
   UNIDENTIFIED                          0.3       *        0.3
     CLASS I  WITH [illegible]                     *
     CLASS II                           0.0        *  0.0
     CLASS III                          0.0        *  0.0
     CLASS IV                           0.3        *  0.0
     CLASS V                            0.0        *  0.0
     CLASS VI                           0.0        *  0.0
     CLASS VII                          0.0        *  0.0
```

```
EMR3E0701.MI   07 [illegible]
1UL EMR TEST SAMPLE #3

                              MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  0.69996



SUM OF PEAK HEIGHTS                 45405900.0
SUM OF DE-ISOTOPED PEAKS            40594300.0

DENSITY OF TEST SAMPLE                    0.9406

AMOUNT OF RECOVERY                      91.0


AVERAGE MOLECULAR WEIGHT               199.9



                                                *
                                                *  ESTIMATED
                                    VOLUME PCT  *  WEIGHT PCT
                                    ----------- *  -----------
  SATURATES                               49.9  *         43.4
     PARAFFINS                      20.3        *  16.4
     NONCOND CYCLOPARAFFINS         13.7        *  11.5
     COND CYCLOPAR 2-RING            7.8        *   6.5
     COND CYCLOPAR 3-RING+           8.7        *   8.5
  AROMATICS                               50.0  *         56.5
   MONO-                             14.5       *      14.1
     BENZENES                        5.0        *   4.6
     NAPHTHENEBENZENES               5.2        *   5.2
     DINAPHTHENEBENZENES             4.3        *   4.3
   DI-                               19.7       *      22.4
     NAPHTHALENES                    5.5        *   5.9
     ACENAPHTHENES, DBZFURANS        7.5        *   8.6
     FLUORENES                       6.7        *   7.9
   TRI-                              8.7        *      11.0
     PHENANTHRENES                   7.6        *   9.5
     NAPHTHENEPHENANTHRENES          1.1        *   1.5
   TETRA-                            1.4        *       1.8
     PYRENES                         1.2        *   1.6
     CHRYSENES                       0.1        *   0.2
   PENTA-                            0.0        *       0.0
     PERYLENES                       0.0        *   0.1
     DIBENZANTHRACENES               0.0        *   0.0
   THIOPHENO-                        5.4        *       7.0
     BENZOTHIOPHENES                 1.4        *   1.6
     DIBENZOTHIOPHENES               3.9        *   5.3
     NAPHTHOBENZOTHIOPHENES          0.1        *   0.1
   UNIDENTIFIED                      0.0        *       0.0
     CLASS I  WITH NAPHPHENAN                   *
     CLASS II                        0.0        *   0.0
     CLASS III                       0.0        *   0.0
     CLASS IV                        0.0        *   0.0
     CLASS V                         0.0        *   0.0
     CLASS VI                        0.0        *   0.0
     CLASS VII                       0.0        *   0.0
```

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EMR3C0701.MI  07/01/86
10% EMR TEST SAMPLE #3

                             MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                    0.17776


SUM OF PEAK HEIGHTS                 32099100.0
SUM OF DE-ISOTOPED PEAKS            17213700.0

DENSITY OF TEST SAMPLE                        0.8429

AMOUNT OF RECOVERY                            44.9

AVERAGE MOLECULAR WEIGHT                     199.9


                                               *
                                               *  ESTIMATED
                                     VOLUME PCT *  WEIGHT PCT
                                     ---------- * -----------
   SATURATES                               49.3 *          42.8
      PARAFFINS                   [illegible]    * 15.8
      NONCOND CYCLOPARAFFINS      [illegible]    *  9.1
      COND CYCLOPAR 2-RING        [illegible]    * 10.8
      COND CYCLOPAR 3-RING+       [illegible]    *  6.7
   AROMATICS                               50.5 *          57.1
    MONO-                             13.9      *      14.4
      BENZENES                    3.1           *  4.5
      NAPHTHENEBENZENES           5.1           *  5.1
      DINAPHTHENEBENZENES         4.5           *  4.5
    DI-                               17.7      *      22.3
      NAPHTHALENES                5.1           *  5.4
      ACENAPHTHENES DIBENZOFURANS 7.8           *  8.9
      FLUORENES                   6.7           *  7.9
    TRI-                               9.0      *      11.3
      PHENANTHRENES               8.0           * 10.1
      NAPHTHENEPHENANTHRENES      0.9           *  1.2
    TETRA-                             1.0      *       1.3
      PYRENES                     0.7           *  0.9
      CHRYSENES                   0.3           *  0.4
    PENTA-                             0.0      *       0.0
      PERYLENES                   0.0           *  0.0
      DIBENZANTHRACENES           0.0           *  0.0
    THIOPHENO-                         5.8      *       7.5
      BENZOTHIOPHENES             1.3           *  1.5
      DIBENZOTHIOPHENES           4.5           *  5.9
      NAPHTHOBENZOTHIOPHENES      0.0           *  0.0
    UNIDENTIFIED                       0.0      *       0.0
      CLASS I  WITH NAPHPHENAN                  *
      CLASS II                    0.0           *  0.0
      CLASS III                   0.0           *  0.0
      CLASS IV                    0.0           *  0.0
      CLASS V                     0.0           *  0.0
      CLASS VI                    0.0           *  0.0
      CLASS VII                   0.0           *  0.0
```

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EMR4A0701 MI  07/01/86
1UL EMR TEST SAMPLE #4

                     MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                0.79799



SUM OF PEAK HEIGHTS                  67370600.0
SUM OF DE-ISOTOPED PEAKS             59044300.0

DENSITY OF TEST SAMPLE                     1.0581

AMOUNT OF RECOVERY                       95.1


AVERAGE MOLECULAR WEIGHT                199.9


                                                *
                                                *  ESTIMATED
                                   VOLUME PCT   *  WEIGHT PCT
                                   ------------ *  -----------
   SATURATES                              17.6  *        13.2
      PARAFFINS                    10.3         *  7.2
      MONOCND CYCLOPARAFFINS        4.8         *  3.7
      COND CYCLOPAR 2-RING          1.8         *  1.5
      COND CYCLOPAR 3-RING+         0.8         *  0.7
   AROMATICS                              82.3  *        86.7
    MONO-                            4.5        *     4.0
      BENZENES                      0.7         *  0.5
      NAPHTHENEBENZENES             2.2         *  1.9
      DINAPHTHENEBENZENES           1.6         *  1.4
    DI-                             41.8        *     42.0
      NAPHTHALENES                 12.7         * 12.0
      ACENAPHTHENES, DBZFURANS     15.3         * 15.6
      FLUORENES                    13.7         * 14.3
    TRI-                            22.8        *     25.6
      PHENANTHRENES                20.9         * 23.4
      NAPHTHENEPHENANTHRENES        1.8         *  2.1
    TETRA-                           1.2        *      1.5
      PYRENES                       1.2         *  1.4
      CHRYSENES                     0.0         *  0.0
    PENTA-                           0.0        *      0.0
      PERYLENES                     0.0         *  0.0
      DIBENZANTHRACENES             0.0         *  0.0
    THIOPHENO-                      11.8        *     13.5
      BENZOTHIOPHENES               2.7         *  2.9
      DIBENZOTHIOPHENES             9.0         * 10.5
      NAPHTHOBENZOTHIOPHENES        0.0         *  0.0
    UNIDENTIFIED                     0.0        *      0.0
      CLASS I  WITH NAPHPHENAN                  *
      CLASS II                      0.0         *  0.0
      CLASS III                     0.0         *  0.0
      CLASS IV                      0.0         *  0.0
      CLASS V                       0.0         *  0.0
      CLASS VI                      0.0         *  0.0
      CLASS VII                     0.0         *  0.0
```

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EMR433[illegible]
1UL EMR TEST SAMPLE #4

                       MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                               0. 79751



SUM OF PEAK HEIGHTS              70582900. 0
SUM OF [illegible] PEAKS         61821400. 0

DENSITY OF TEST SAMPLE                 1. 0537

AMOUNT OF RECOVERY                    96. 4


AVERAGE MOLECULAR WEIGHT             199 9


                                                  *
                                                  *  ESTIMATED
                                    VOLUME PCT    *  WEIGHT PCT
                                   ------------   *  ------------
 SATURATES                                15. [illegible] *          12. 4
    PARAFFINS                       9. 1          *   6. 5
    NONCONDENSED CYCLOPARAFFINS     4 0           *   3 1
    CONDENSED CYCLOPARAFFIN 2-RING  3 4           *   2. 0
    CONDENSED CYCLOPARAFFIN 3-RING+ 0 7           *   0. 6
 AROMATICS                         [illegible]    *          87. 5
  MONO-                                  5. 3     *       5. 1
    BENZENES                        0 9           *   0. 7
    NAPHTHENEBENZENES               2 8           *   2. 5
    DINAPHTHENEBENZENES             2 0           *   1 8
  DI-                                   45 2      *      45. 6
    NAPHTHALENES                   15. 1          *  14 3
    ACENAPHTHENES DIBENZFURANS     17 2           *  17 7
    FLUORENES                      12. 8          *  13 5
  TRI-                                  20. 9     *      23 4
    PHENANTHRENES                  19 3           *  21 7
    NAPHTHENE PHENANTHRENES         1. 5          *   1 7
  TETRA-                                 1 2      *       1. 5
    PYRENES                         1 2              1. 4
    CHRYSENES                       0. 0          *   0. 0
  PENTA-                                 0. 0     *       0. 0
    PERYLENES                       0 0           *   0. 0
    DIBENZANTHRACENES               0 0           *   0 0
  THIOPHENO-                            10. 2     *      11 8
    BENZOTHIOPHENES                 2 5           *   2 7
    DIBENZOTHIOPHENES               7 5           *   8 9
    NAPHTHOBENZOTHIOPHENES          0 1           *   0 2
  UNIDENTIFIED                           0. 0     *       0. 0
    CLASS I  WITH NAPHPHENAN                      *
    CLASS II                        0. 0          *   0 0
    CLASS III                       0. 0          *   0 0
    CLASS IV                        0 0           *   0. 0
    CLASS V                         0. 0          *   0. 0
    CLASS VI                        0. 0          *   0. 0
    CLASS VII                       0 0           *   0 0
```

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EMR4C0701.M1 [illegible]
1UL EMR TEST SAMPLE #4

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                    0.79761


SUM OF PEAK HEIGHTS                   66397700.0
SUM OF [illegible] PEAKS              58377300.0

DENSITY OF TEST SAMPLE                     1.0352

AMOUNT OF RECOVERY                         94.9

AVERAGE MOLECULAR WEIGHT                  199.9


                                                   *
                                                   *  ESTIMATED
                                      VOLUME PCT   *  WEIGHT PCT
                                      ------------ *  -----------
   SATURATES                                 17.6  *          13.4
      PARAFFINS                       11.0         *  8.1
      NONCOND CYCLOPARAFFINS           3.7         *  2.9
      COND CYCLOPAR 2-RING             2.2         *  1.8
      COND CYCLOPAR 3-RING+            0.5         *  0.5
   AROMATICS                                 82.1  *          86.5
    MONO-                                6.7       *       5.9
      BENZENES                         2.0         *  1.6
      NAPHTHENEBENZENES                2.6         *  2.3
      DINAPHTHENEBENZENES              2.1         *  1.9
    DI-                                 50.3       *      51.4
      NAPHTHALENES                    18.4         * 17.7
      ACENAPHTHENES DIBENZOFURANS     19.6         * 20.4
      FLUORENES                       12.3         * 13.2
    TRI-                                16.4       *      18.7
      PHENANTHRENES                   15.8         * 18.0
      NAPHTHENOPHENANTHRENES           0.6         *  0.7
    TETRA-                               0.5       *       0.6
      PYRENES                          0.5         *  0.5
      CHRYSENES                        0.0         *  0.0
    PENTA-                               0.0       *       0.0
      PERYLENES                        0.0         *  0.0
      DIBENZANTHRACENES                0.0         *  0.0
    THIOPHENO-                           8.2       *       9.6
      BENZOTHIOPHENES                  2.2         *  2.4
      DIBENZOTHIOPHENES                6.0         *  7.1
      NAPHTHOBENZOTHIOPHENES           0.0         *  0.0
    UNIDENTIFIED                         0.0       *       0.0
      CLASS I [illegible] NAPHPHENAN               *
      CLASS II                         0.0         *  0.0
      CLASS III                        0.0         *  0.0
      CLASS IV                         0.0         *  0.0
      CLASS V                          0.0         *  0.0
      CLASS VI                         0.0         *  0.0
      CLASS VII                        0.0         *  0.0
```

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EMR50701A MI  07/01/86
1UL EMR TEST SAMPLE #5

                        MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.69996


SUM OF PEAK HEIGHTS                55949900.0
SUM OF DE-ISOTOPED PEAKS           50567200.0

DENSITY OF TEST SAMPLE                   0.9016

AMOUNT OF RECOVERY                       86.5

AVERAGE MOLECULAR WEIGHT                199.9

                                              *
                                              *  ESTIMATED
                                  VOLUME PCT  *  WEIGHT PCT
                                 ------------ * ------------
    SATURATES                           59.5  *        54.2
       PARAFFINS                 20.6         * 17.4
       NONCOND CYCLOPARAFFINS    17.5         * 15.7
       COND CYCLOPAR 2-RING      11.5         * 11.1
       COND CYCLOPAR 3-RING+      9.7         *  9.9
    AROMATICS                           40.4  *        45.7
     MONO-                        17.8        *      18.0
       BENZENES                   5.8         *  5.6
       NAPHTHENEBENZENES          4.9         *  5.2
       DINAPHTHENEBENZENES        7.1         *  7.2
     DI-                          14.4        *      16.9
       NAPHTHALENES               6.4         *  6.7
       ACENAPHTHENES, DBZFURANS   4.1         *  5.3
       FLUORENES                  3.9         *  4.8
     TRI-                          2.7        *       3.6
       PHENANTHRENES              2.0         *  2.7
       NAPHTHENEPHENANTHRENES     0.6         *  0.9
     TETRA-                        0.8        *       1.1
       PYRENES                    0.6         *  0.9
       CHRYSENES                  0.1         *  0.2
     PENTA-                        0.0        *       0.0
       PERYLENES                  0.0         *  0.0
       DIBENZANTHRACENES          0.0         *  0.0
     THIOPHENO-                    4.5        *       5.9
       BENZOTHIOPHENES            3.3         *  4.2
       DIBENZOTHIOPHENES          1.2         *  1.7
       NAPHTHOBENZOTHIOPHENES     0.0         *  0.0
     UNIDENTIFIED                  0.0        *       0.0
       CLASS I  WITH NAPHPHENAN               *
       CLASS II                   0.0         *  0.0
       CLASS III                  0.0         *  0.0
       CLASS IV                   0.0         *  0.0
       CLASS V                    0.0         *  0.0
       CLASS VI                   0.0         *  0.0
       CLASS VII                  0.0         *  0.0
```

```
EMR50701B.MI  07/01/86
1UL EMR TEST SAMPLE #3

                          MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  [illegible]9996



SUM OF PEAK HEIGHTS                 55975200.0
SUM OF DE-ISOTOPED PEAKS            50567900.0

DENSITY OF TEST SAMPLE                    0.9027

AMOUNT OF RECOVERY                       96.2


AVERAGE MOLECULAR WEIGHT                199.[illegible]



                                                  *
                                                  *  ESTIMATED
                                     VOLUME PCT   *  WEIGHT PCT
                                     ----------   *  -----------
   SATURATES                                59.3  *          54.1
      PARAFFINS                     [illegible]   * 16.5
      NONCOND CYCLOPARAFFINS        [illegible]   * 15.2
      COND CYCLOPAR 2-RING          [illegible]   * 12.7
      COND CYCLOPAR 3-RING+         [illegible]   *  9.5
   AROMATICS                                40.6  *          45.8
    MONO-                              17.9       *      19.1
      BENZENES                      [illegible]   *  5.4
      NAPHTHENEBENZENES             [illegible]   *  5.5
      DINAPHTHENEBENZENES           [illegible]   *  7.2
    DI-                                14.5       *      17.0
      NAPHTHALENES                  6.2           *  6.8
      ACENAPHTHENES/DIBENZOFURANS   4.6           *  5.5
      FLUORENES                     3.7           *  4.5
    TRI-                               3.7        *       3.6
      PHENANTHRENES                 3.1           *  2.8
      NAPHTHENEPHENANTHRENES        0.6           *  0.8
    TETRA-                             0.7        *       0.9
      PYRENES                       0.6           *  0.9
      CHRYSENES                     0             *  0.0
    PENTA-                             0.0        *       0.0
      PERYLENES                     0.0           *  0.0
      DIBENZANTHRACENES             0.0              0
    THIOPHENO-                      [illegible]   *       5.9
      BENZOTHIOPHENES                             *  4.0
      DIBENZOTHIOPHENES             1.3           *  1.7
      NAPHTHOBENZOTHIOPHENES        0.0           *  0.0
    UNIDENTIFIED                       0.0        *       0.0
      CLASS I  WITH NAP[illegible]                *
      CLASS II                      0.0           *  0.0
      CLASS III                     0.0           *  0.0
      CLASS IV                      0.0           *  0.0
      CLASS V                       0.0           *  0.0
      CLASS VI                      0.0           *  0.0
      CLASS VII                     [illegible]   *  0.0
```

```
EMC50701C.MI  07/01/86
1UL EMR TEST SAMPLE #5

                       MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  0.69996



SUM OF PEAK HEIGHTS               58837500.0
SUM OF DE-ISOTOPED PEAKS          53166700.0

DENSITY OF TEST SAMPLE                      0.9033

AMOUNT OF RECOVERY                         85.4


AVERAGE MOLECULAR WEIGHT                  199.9



                                                 *
                                                 *  ESTIMATED
                                    VOLUME PCT   *  WEIGHT PCT
                                    ------------ *  ------------
   SATURATES                                59.1 *          53.9
      PARAFFINS                     19.4         * 16.3
      NONCOND CYCLOPARAFFINS        17.2         * 15.4
      COND CYCLOPAR 2-RING          13.0         * 12.5
      COND CYCLOPAR 3-RING+          9.3         *  9.5
   AROMATICS                                40.8 *          46.0
    MONO-                              17.9      *     18.1
      BENZENES                       5.6         *  5.3
      NAPHTHENEBENZENES              5.3         *  5.6
      DINAPHTHENEBENZENES            6.9         *  7.1
    DI-                                14.7      *     17.1
      NAPHTHALENES                   6.2         *  6.8
      ACENAPHTHENES, DIBFURANS       4.5         *  5.4
      FLUORENES                      3.9         *  4.7
    TRI-                                2.5      *      3.4
      PHENANTHRENES                  2.0         *  2.6
      NAPHTHENEPHENANTHRENES         0.5         *  0.7
    TETRA-                              0.7      *      1.0
      PYRENES                        0.6         *  0.8
      CHRYSENES                      0.1         *  0.1
    PENTA-                              0.0      *      0.0
      PERYLENES                      0.0         *  0.0
      DIBENZANTHRACENES              0.0         *  0.0
    THIOPHENO-                          4.7      *      6.1
      BENZOTHIOPHENES                3.4         *  4.3
      DIBENZOTHIOPHENES              1.3         *  1.7
      NAPHTHOBENZOTHIOPHENES         0.0         *  0.0
    UNIDENTIFIED                        0.0      *      0.0
      CLASS I  WITH NAPHPHENAN                   *
      CLASS II                       0.0         *  0.0
      CLASS III                      0.0         *  0.0
      CLASS IV                       0.0         *  0.0
      CLASS V                        0.0         *  0.0
      CLASS VI                       0.0         *  0.0
      CLASS VII                      0.0         *  0.0
```

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EMPE0702A MI  07/02/86
1UL EMR TEST SAMPLE #6

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.69996



SUM OF PEAK HEIGHTS               71094100.0
SUM OF DE-ISOTOPED PEAKS          63822500.0

DENSITY OF TEST SAMPLE                     0.9268

AMOUNT OF RECOVERY                       83.9


AVERAGE MOLECULAR WEIGHT                199.9



                                                *
                                                *  ESTIMATED
                                    VOLUME PCT  *  WEIGHT PCT
                                   ------------ * ------------
   SATURATES                              57.3  *         52.2
      PARAFFINS                     8.2         *  6.7
      NONCOND CYCLOPARAFFINS       18.8         * 16.4
      COND CYCLOPAR 2-RING         18.7         * 17.5
      COND CYCLOPAR 3-RING+        11.5         * 11.4
   AROMATICS                              42.6  *         47.7
    MONO-                            17.1       *      17.1
      BENZENES                      2.7         *  2.5
      NAPHTHENEBENZENES             5.9         *  6.0
      DINAPHTHENEBENZENES           8.4         *  8.5
    DI-                              14.8       *      17.0
      NAPHTHALENES                  4.3         *  4.7
      ACENAPHTHENES, DBZFURANS      5.4         *  6.3
      FLUORENES                     4.9         *  5.9
    TRI-                              3.8       *       4.8
      PHENANTHRENES                 2.9         *  3.7
      NAPHTHENEPHENANTHRENES        0.8         *  1.1
    TETRA-                            1.1       *       1.5
      PYRENES                       0.9         *  1.3
      CHRYSENES                     0.1         *  0.2
    PENTA-                            0.0       *       0.0
      PERYLENES                     0.0         *  0.0
      DIBENZANTHRACENES             0.0         *  0.0
    THIOPHENO-                        5.6       *       7.0
      BENZOTHIOPHENES               4.6         *  5.6
      DIBENZOTHIOPHENES             1.0         *  1.3
      NAPHTHOBENZOTHIOPHENES        0.0         *  0.0
    UNIDENTIFIED                      0.0       *       0.0
      CLASS I  WITH NAPHPHENAN                  *
      CLASS II                      0.0         *  0.0
      CLASS III                     0.0         *  0.0
      CLASS IV                      0.0         *  0.0
      CLASS V                       0.0         *  0.0
      CLASS VI                      0.0         *  0.0
      CLASS VII                     0.0         *  0.0
```

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[illegible]
IOL SUR TEST SAMPLE [illegible]

                          MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                     0 69996



SUM OF PEAK HEIGHTS                 74519100 0
SUM OF DE-ISOTOPED PEAKS            [illegible]000 0

DENSITY OF TEST SAMPLE                    0 9372

AMOUNT OF RECOVERY                       [illegible] 0

AVERAGE MOLECULAR WEIGHT                 [illegible] 9



                                                 *
                                                 *  ESTIMATED
                                    VOLUME PCT   *  WEIGHT PCT
                                    ----------   *  -----------
   SATURATES                             57 0    *          51 9
      PARAFFINS                     5 4          *  6 9
      NONCOND CYCLOPARAFFINS        12 9         *  16 5
      COND CYCLOPARAFFINS           17 3         *  16 7
      COND [illegible]              11 [illegible] *  11 5
   AROMATICS                             43 [illegible] *   48 0
    MONO-                           17 1         *       17 1
      BENZENES                      [illegible]  *  7 6
      NAPHTHENEBENZENES             5 [illegible] *  5 7
      DINAPHTHENEBENZENES           3 4          *  3 6
    DI-                                11 9      *       17 1
      NAPHTHALENES                  3 4          *  4 3
      ACENAPHTHENES,DIBENZOFURANS   3 4          *  [illegible]
      FLUORENES                     5.0          *  6 0
    TRI-                               3 8       *        4 9
      PHENANTHRENES                 2 9          *  3 5
      NAPHTHENOPHENANTHRENES        0 9          *  1 2
    TETRA-                             1 1       *        1 5
      PYRENES                       0 9          *  1 3
      CHRYSENES                     0 1          *  0 2
    PENTA-                             0 0       *        0 0
      PERYLENES                     0 0          *  0.0
      DIBENZANTHRACENES             0 0          *  0 0
    THIOPHENO-                         5 0       *        7 2
      BENZOTHIOPHENES               4 0          *  5 [illegible]
      DIBENZOTHIOPHENES             1 0          *  1 3
      NAPHTHOBENZOTHIOPHENES        0 0          *  0 0
    UNIDENTIFIED                       0 0       *        0 0
      CLASS I  [illegible]                       *
      CLASS II                      0 0          *  0.0
      CLASS III                     0.0          *  0 0
      CLASS IV                      0 0          *  0.0
      CLASS V                       0 0          *  0.0
      CLASS VI                      0.0          *  0 0
      CLASS VII                     0 0          *  0.0
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EMR607020 MI  07/02/86
1UL EMR TEST SAMPLE #6

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.59996



SUM OF PEAK HEIGHTS                83486000.0
SUM OF DE-ISOTOPED PEAKS           74927600.0

DENSITY OF TEST SAMPLE                     0.9287

AMOUNT OF RECOVERY                        92.6


AVERAGE MOLECULAR WEIGHT                 199.9



                                                   *
                                                   *  ESTIMATED
                                       VOLUME PCT  *  WEIGHT PCT
                                      ------------ * ------------
   SATURATES                                  56.0 *          50.9
      PARAFFINS                        9.8         *  8.0
      NONCOND CYCLOPARAFFINS          17.3         * 15.0
      COND CYCLOPAR 2-RING            13.9         * 14.9
      COND CYCLOPAR 3-RING+           12.9         * 12.7
   AROMATICS                                  43.9 *          49.0
    MONO-                                17.5      *       17.5
      BENZENES                         3.1         *  2.9
      NAPHTHENEBENZENES                5.7         *  5.8
      DINAPHTHENEBENZENES              8.6         *  8.7
    DI-                                  15.3      *       17.6
      NAPHTHALENES                     4.4         *  4.8
      ACENAPHTHENES, DBZFURANS         5.4         *  6.3
      FLUORENES                        5.3         *  6.4
    TRI-                                  3.3      *        4.3
      PHENANTHRENES                    2.5         *  3.2
      NAPHTHENEPHENANTHRENES           0.8         *  1.0
    TETRA-                                1.3      *        1.7
      PYRENES                          1.1         *  1.4
      CHRYSENES                        0.2         *  0.2
    PENTA-                                0.0      *        0.0
      PERYLENES                        0.0         *  0.0
      DIBENZANTHRACENES                0.0         *  0.0
    THIOPHENO-                            6.2      *        7.7
      BENZOTHIOPHENES                  5.0         *  6.0
      DIBENZOTHIOPHENES                1.1         *  1.5
      NAPHTHOBENZOTHIOPHENES           0.1         *  0.1
    UNIDENTIFIED                          0.0      *        0.0
      CLASS I  WITH NAPHPHENAN                     *
      CLASS II                         0.0         *  0.0
      CLASS III                        0.0         *  0.0
      CLASS IV                         0.0         *  0.0
      CLASS V                          0.0         *  0.0
      CLASS VI                         0.0         *  0.0
      CLASS VII                        0.0         *  0.0
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EMR11A0701 MI [illegible]
1UL EMR TEST SAMPLE #11

                          MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                              0 59999


SUM OF PEAK HEIGHTS                34167000 0
SUM OF DE-ISOTOPED PEAKS           31453600 0

DENSITY OF TEST SAMPLE                  0 8608

AMOUNT OF RECOVERY                     79 1

AVERAGE MOLECULAR WEIGHT              199 7



                                                  *
                                                  *  ESTIMATED
                                     VOLUME PCT   *  WEIGHT PCT
                                     ------------ *  ------------
  SATURATES                                [illegible] 1  *          85. 1
    PARAFFINS                        [illegible]          *  15 3
    NONCOND CYCLOPARAFFINS           [illegible]          *  32 4
    COND 2 CYCLOPAR RINGS            [illegible]          *  23 8
    COND 3 CYCLOPAR RINGS+           [illegible]          *  13 4
  AROMATICS                                11 9  *          14. 8
   MONO-                                3 5      *         3 8
    BENZENES                         [illegible]          *  0 0
    NAPHTHENOBENZENES                [illegible]          *  0 7
    DINAPHTHENOBENZENES              [illegible]          *  [illegible] 1
   DI-                                  5 0      *         6. 3
    NAPHTHALENES                     [illegible]          *  [illegible] 3
    ACENAPHTHENES DIBENZOFURANS      [illegible]          *  1 5
    FLUORENES                        [illegible]          *  [illegible] 3
   TRI-                                 [illegible] 2      *         3. 1
    PHENANTHRENES                    [illegible]          *  [illegible] 8
    NAPHTHENOPHENANTHRENES           [illegible]          *  0 2
   TETRA-                               0 4      *         0 7
    PYRENES                          [illegible]          *  [illegible]
    CHRYSENES                        [illegible]          *  [illegible]
   PENTA-                               0 0      *         0 0
    PERYLENES                        [illegible]          *  0. 0
    DIBENZANTHRACENES                [illegible]          *  0 0
   THIOPHENO-                           0 5      *         0 7
    BENZOTHIOPHENES                  [illegible]          *  0 4
    DIBENZOTHIOPHENES                [illegible]          *  0 2
    NAPHTHOBENZOTHIOPHENES           [illegible]          *  0 0
  UNIDENTIFIED                          0 0      *         0. 0
    CLASS I  WITH NAPHPHENAN                      *
    CLASS II                         0 0          *  0. 0
    CLASS III                        0 0          *  0. 0
    CLASS IV                         0 0          *  0 0
    CLASS V                          0 0          *  0. 0
    CLASS VI                         0 0          *  0 0
    CLASS VII                        0 0          *  0 0
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EMR1180701.MI  07/01/86
1UL EMR TEST SAMPLE #11

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  0.57839


SUM OF PEAK HEIGHTS               3088[illegible].0
SUM OF DE-ISOTOPED PEAKS          31249200.0

DENSITY OF TEST SAMPLE                      0.8508

AMOUNT OF RECOVERY                          0.0


AVERAGE MOLECULAR WEIGHT                  [illegible]



                                                 *
                                                 *  ESTIMATED
                                     VOLUME PCT  *  WEIGHT PCT
                                  -------------  *  -----------
   SATURATES                               88.3  *          85.3
      PARAFFINS                     15.4         *  14.5
      NONCOND CYCLOPARAFFINS        36.2         *  34.1
      COND CYCLOPAR 2-RING          [illegible]  *  23.6
      COND CYCLOPAR 3-RING+         12.1         *  12.9
   AROMATICS                               11.6  *          14.6
    MONO-                             3.4        *       3.7
      BENZENES                      0.0          *  0.0
      NAPHTHENEBENZENES             0.6          *  0.6
      DINAPHTHENEBENZENES           2.7          *  3.0
    DI-                               4.7        *       6.1
      NAPHTHALENES                  0.1          *  0.1
      ACENAPHTHENES, DBZFURANS      1.2          *  1.5
      FLUORENES                     3.3          *  [illegible]
    TRI-                              2.6        *       3.0
      PHENANTHRENES                 [illegible]  *  [illegible]
      NAPHTHENEPHENANTHRENES        0.1          *  0.2
    TETRA-                            0.5        *       0.7
      PYRENES                       0.1          *  [illegible]
      CHRYSENES                     0.0          *  0.0
    PENTA-                            0.0        *       0.0
      PERYLENES                     [illegible]  *  0.0
      DIBENZANTHRACENES             0.0          *  0.0
    THIOPHENO-                        0.7        *       0.9
      BENZOTHIOPHENES               [illegible]  *  [illegible]
      DIBENZOTHIOPHENES             [illegible]  *  0.3
      NAPHTHOBENZOTHIOPHENES        [illegible]  *  0.1
    UNIDENTIFIED                      0.0        *       0.0
      CLASS I  WITH NAPHPHENAN                   *
      CLASS II                      0.0          *  0.0
      CLASS III                     0.0          *  0.0
      CLASS IV                      0.0          *  0.0
      CLASS V                       0.0          *  0.0
      CLASS VI                      0.0          *  0.0
      CLASS VII                     0.0          *  0.0
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EMR110701 MI 07/01/86
1UL EMR TEST SAMPLE #11

                    MASS SPECTRAL ANALYSIS OF [illegible]
AIN FACTOR                                      0 59839



SUM OF PEAK HEIGHTS                  [illegible]2479000. 0
SUM OF DE-ISOTOPED PEAKS             2791[illegible]200. 0

DENSITY OF TEST SAMPLE                          0 8610

AMOUNT OF RECOVERY                              78. 2


AVERAGE MOLECULAR WEIGHT                        199. 9



                                                    *
                                                    *  ESTIMATED
                                       [illegible]ME PCT  *  WEIGHT PCT
                                         ---------  *  ------------
    SATURATES                                88. 1  *          85. 1
      PARAFFINS                   [illegible]       *  14. 4
      NONCOND CYCLOPARAFFINS      [illegible]       *  34. 0
      COND CYCLOPAR 2-RING        [illegible]       *  23. 8
      COND CYCLOPAR 3-RING+       11. -             *  12. 7
    AROMATICS                                11. 8  *          14. 8
     MONO-                               3. 5       *       3. 8
      BENZENES                    0. 0              *   0. 0
      NAPHTHENEBENZENES                             *   0. 7
      DINAPHTHENEBENZENES         [illegible]       *   3. 1
     DI-                                 [illegible]*       6. 1
      NAPHTHALENES                0. 1              *   0. 2
      ACENAPHTHENES, DBZFURANS    [illegible]       *   1. 5
      FLUORENES                   [illegible]       *   4. 3
     TRI-                                [illegible]*       3. 1
      PHENANTHRENES               [illegible]       *   2 9
      NAPHTHENEPHENANTHRENES      0. 1              *   0. 2
     [illegible]                         0. 4       *       0. 6
      [illegible]                 0. 4              *   0. 6
      [illegible]                 0. 0              *   0. 0
     PENTA-                              0. 0       *       0. 0
      PERYLENES                   0. 0              *   0. 0
      DIBENZANTHRACENES           0 0               *   0. 0
     THIOPHENO-                          0. 6       *       0 9
      BENZOTHIOPHENES             0. 3              *   0 4
      DIBENZOTHIOPHENES           0 2               *   0. 3
      NAPHTHOBENZOTHIOPHENES      0. 0              *   0. 1
     UNIDENTIFIED                        0. 0       *       0. 0
      CLASS I  WITH NAPHPHENAN                      *
      CLASS II                    0. 0              *   0. 0
      CLASS III                   0. 0              *   0. 0
      CLASS IV                    0 0               *   0. 0
      CLASS V                     0. 0              *   0. 0
      CLASS VI                    0. 0              *   0. 0
      CLASS VII                   0. 0              *   0. 0
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MS499141A.MI  06/27/86
[illegible] MB-499-141

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59539



SUM OF PEAK HEIGHTS              6718830.0
SUM OF DE-ISOTOPED PEAKS         6204890.0

DENSITY OF TEST SAMPLE                 0.8524

AMOUNT OF RECOVERY                   101.0


AVERAGE MOLECULAR WEIGHT             179.9


                                             *
                                             *  ESTIMATED
                                 VOLUME PCT  *  WEIGHT PCT
                                 ----------  *  ----------
  SATURATES                            91.9  *          89.8
    PARAFFINS                  18.5          *  16.5
    NONCOND CYCLOPARAFFINS     33.5          *  31.9
    COND CYCLOPAR 2-RING       26.9          *  27.4
    COND CYCLOPAR 3-RING+      12.9          *  13.9
  AROMATICS                             8.0  *          10.1
  MONO-                          2.2         *       2.5
    BENZENES                    0.0          *   0.0
    NAPHTHENEBENZENES           0.7          *   0.8
    DINAPHTHENEBENZENES         1.5          *   1.7
  DI-                            3.2         *       4.2
    NAPHTHALENES                0.2          *   0.2
    ACENAPHTHENES, DBZFURANS    0.9          *   1.1
    FLUORENES                   2.1          *   2.8
  TRI-                           1.5         *       2.2
    PHENANTHRENES               1.4          *   2.0
    NAPHTHENEPHENANTHRENES      0.1          *   0.1
  TETRA-                         0.3         *       0.5
    PYRENES                     0.3          *   0.4
    CHRYSENES                   0.0          *   0.0
  PENTA-                         0.0         *       0.0
    PERYLENES                   0.0          *   0.0
    DIBENZANTHRACENES           0.0          *   0.0
  THIOPHENO-                     0.3         *       0.4
    BENZOTHIOPHENES             0.2          *   0.3
    DIBENZOTHIOPHENES           0.0          *   0.0
    NAPHTHOBENZOTHIOPHENES      0.0          *   0.0
  UNIDENTIFIED                   0.0         *       0.0
    CLASS I  WITH NAPHPHENAN                 *
    CLASS II                    0.0          *   0.0
    CLASS III                   0.0          *   0.0
    CLASS IV                    0.0          *   0.0
    CLASS V                     0.0          *   0.0
    CLASS VI                    0.0          *   0.0
    CLASS VII                   0.0          *   0.0
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MB4991413.MI  06/21/..
1UL MB-499-141

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.89879



SUM OF PEAK HEIGHTS             4722990.0
SUM OF DE-ISOTOPED PEAKS        4357390.0

DENSITY OF TEST SAMPLE                0.8546

AMOUNT OF RECOVERY                  99.4


AVERAGE MOLECULAR WEIGHT           199.9



                                               *
                                               *  ESTIMATED
                                    VOLUME PCT *  WEIGHT PCT
                                    ---------- *  ----------
   SATURATES                              91.8 *        89.8
     PARAFFINS                   17.7          *  15.1
     NONCOND CYCLOPARAFFINS      33.5          *  31.8
     COND CYCLOPAR 2-RING        27.4          *  27.7
     COND CYCLOPAR 3-RING        13.2          *  14.9
   AROMATICS                               8.1 *        10.1
    MONO-                            2.4       *       2.6
     BENZENES                     0.0          *   0.0
     NAPHTHENEBENZENES            0.8          *   0.9
     DINAPHTHENEBENZENES          1.5          *   1.7
    DI-                              3.3       *       4.2
     NAPHTHALENES                 0.1          *   0.2
     ACENAPHTHENES, DBZFURANS     0.9          *   1.1
     FLUORENES                    2.2          *   2.9
    TRI-                             1.7       *       2.4
     PHENANTHRENES                1.6          *   2.2
     NAPHTHENEPHENANTHRENES       0.1          *   0.1
    TETRA-                           0.2       *       0.3
     PYRENES                      0.2          *   0.3
     CHRYSENES                    0.0          *   0.0
    PENTA-                           0.0       *       0.0
     PERYLENES                    0.0          *   0.0
     DIBENZANTHRACENES            0.0          *   0.0
    THIOPHENO-                       0.3       *       0.4
     BENZOTHIOPHENES              0.2          *   0.3
     DIBENZOTHIOPHENES            0.1          *   0.1
     NAPHTHOBENZOTHIOPHENES       0.0          *   0.0
    UNIDENTIFIED                     0.0       *       0.0
     CLASS I  WITH NAPHPHENAN                  *
     CLASS II                     0.0          *   0.0
     CLASS III                    0.0          *   0.0
     CLASS IV                     0.0          *   0.0
     CLASS V                      0.0          *   0.0
     CLASS VI                     0.0          *   0.0
     CLASS VII                    0.0          *   0.0
```

```
MB499141C.MI  06/27/86
1UL MB-499-141

                              MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                     0.59839


SUM OF PEAK HEIGHTS                 6252870.0
SUM OF DE-ISOTOPED PEAKS            5779950.0

DENSITY OF TEST SAMPLE                   0.8531

AMOUNT OF RECOVERY                    [illegible]

AVERAGE MOLECULAR WEIGHT              [illegible]


                                                  *
                                                  *  ESTIMATED
                                    VOLUME PCT    *  WEIGHT PCT
                                    ------------- *  -------------
  SATURATES                                 92.0  *          [illegible]
     PARAFFINS                      [illegible]   *  [illegible]
     NONCOND CYCLOPARAFFINS         [illegible]   *  [illegible]
     COND CYCLOPAR 2-RING           [illegible]   *  [illegible]
     COND CYCLOPAR 3-RING+          [illegible]   *  [illegible]
  AROMATICS                                 [illegible] *    [illegible]
   MONO-                                    [illegible] *    [illegible]
     BENZENES                       0.0           *  [illegible]
     NAPHTHENEBENZENES              [illegible]   *  [illegible]
     DINAPHTHENEBENZENES            [illegible]   *  [illegible]
   DI-                                      [illegible] *    [illegible]
     NAPHTHALENES                   0.1           *  0.2
     ACENAPHTHENES/DBZFURANS        0.9           *  1.1
     FLUORENES                      [illegible]   *  [illegible]
   TRI-                                      1.6  *          [illegible]
     PHENANTHRENES                  [illegible]   *  [illegible]
     NAPHTHENOPHENANTHRENES         [illegible]   *  [illegible]
   TETRA-                                    0.3  *          0.4
     PYRENES                        0.3           *  0.1
     CHRYSENES                      0.0           *  0.0
   PENTA-                                    0.0  *          0.0
     PERYLENES                      [illegible]   *  0.0
     DIBENZANTHRACENES              [illegible]   *  0.0
   THIOPHENO-                                0.3  *          0.4
     BENZOTHIOPHENES                0.2           *  [illegible]
     DIBENZOTHIOPHENES              [illegible]   *  [illegible]
     NAPHTHOBENZOTHIOPHENES         [illegible]   *  [illegible]
   UNIDENTIFIED                              0.0  *          0.0
     CLASS I  WITH NAPHPHENAN                     *
     CLASS II                       [illegible]   *  0.0
     CLASS III                      [illegible]   *  0.0
     CLASS IV                       [illegible]   *  0.0
     CLASS V                        [illegible]   *  0.0
     CLASS VI                       0.0           *  0.0
     CLASS VII                      0.0           *  0.0
```

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ME499143A MI [illegible]
1UL ME-499-143

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                   0.59839


SUM OF PEAK HEIGHTS                  7897580.0
SUM OF DE-ISOTOPED PEAKS             7278480.0

DENSITY OF TEST SAMPLE                  0.8598

AMOUNT OF RECOVERY                    101.1


AVERAGE MOLECULAR WEIGHT              199.9



                                                  *
                                                  *  ESTIMATED
                                      VOLUME PCT  *  WEIGHT PCT
                                     ------------ *  ------------
   SATURATES                                88.0  *          85.4
      PARAFFINS                      13.1         *  15.0
      NONCOND CYCLOPARAFFINS         30.7         *  28.9
      COND CYCLOPAR [illegible]      35.3         *  35.6
      COND CYCLOPAR [illegible]      13.8         *  14.3
   AROMATICS                                11.9  *          14.5
    MONO-                               5.3       *       5.8
      BENZENES                        0.2         *   0.2
      NAPHTHENEBENZENES               2.3         *   2.6
      DINAPHTHENEBENZENES             2.7         *   3.0
    DI-                            [illegible]    *       3.9
      NAPHTHALENES                 [illegible]
      ACENAPHTHENES, DIBENZOFURANS [illegible]
      FLUORENES                       2.0
    TRI-                                1.7       *
      PHENANTHRENES                   1.3         *   1
      NAPHTHENEPHENANTHRENES          0.4         *
    TETRA-                         [illegible]           [illegible]
      PYRENES                      [illegible]        0.4
      CHRYSENES                    [illegible]        [illegible]
    PENTA-                                        *
      PERYLENES
      DIBENZANTHRACENES            [illegible]    *   0.0
    THIOPHENO-                          1.3       *       1.7
      BENZOTHIOPHENES                 1.1         *   1.[illegible]
      DIBENZOTHIOPHENES               0.1         *   0.1
      NAPHTHOBENZOTHIOPHENES       [illegible]    *   0.0
    UNIDENTIFIED                        0.0       *       0.0
      CLASS I  WITH NAPHPHENAN                    *
      CLASS II                        0.0         *   0.0
      CLASS III                       0.0         *   0.0
      CLASS IV                        0.0         *   0.0
      CLASS V                         0.0         *   0.0
      CLASS VI                        0.0         *   0.0
      CLASS VII                       0.0         *   0.0
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MB4991438.MI  06/27/86
1UL MB-499-143

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.59839



SUM OF PEAK HEIGHTS               6926140.0
SUM OF DE-ISOTOPED PEAKS          6380320.0

DENSITY OF TEST SAMPLE                0.8617

AMOUNT OF RECOVERY                  99.2


AVERAGE MOLECULAR WEIGHT            199.9



                                                 *
                                                 *  ESTIMATED
                                     VOLUME PCT  *  WEIGHT PCT
                                     ----------- *  -----------
   SATURATES                              87.9   *        85.3
      PARAFFINS                     16.9         * 14.9
      NONCOND CYCLOPARAFFINS        31.0         * 29.1
      COND CYCLOPAR 2-RING          25.4         * 25.6
      COND CYCLOPAR 3-RING+         14.5         * 15.4
   AROMATICS                              12.0   *        14.6
    MONO-                             5.3        *      5.8
      BENZENES                       0.1         *  0.1
      NAPHTHENEBENZENES              2.3         *  2.5
      DINAPHTHENEBENZENES            2.8         *  3.1
    DI-                               3.0        *      3.8
      NAPHTHALENES                   0.3         *  0.1
      ACENAPHTHENES,DBZFURANS        0.8         *  1.0
      FLUORENES                      2.0         *  2.6
    TRI-                              1.7        *      2.4
      PHENANTHRENES                  1.3         *  1.8
      NAPHTHENEPHENANTHRENES         0.4         *  0.6
    TETRA-                            0.3        *      0.5
      PYRENES                        0.3         *  0.4
      CHRYSENES                      0.0         *  0.0
    PENTA-                            0.0        *      0.0
      PERYLENES                      0.0         *  0.0
      DIBENZANTHRACENES              0.0         *  0.0
    THIOPHENO-                        1.5        *      2.0
      BENZOTHIOPHENES                1.2         *  1.7
      DIBENZOTHIOPHENES              0.1         *  0.2
      NAPHTHOBENZOTHIOPHENES         0.0         *  0.0
    UNIDENTIFIED                      0.0        *      0.0
      CLASS I  WITH NAPHPHENAN                   *
      CLASS II                       0.0         *  0.0
      CLASS III                      0.0         *  0.0
      CLASS IV                       0.0         *  0.0
      CLASS V                        0.0         *  0.0
      CLASS VI                       0.0         *  0.0
      CLASS VII                      0.0         *  0.0
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MB499143C MI 08/27/86
1UL MB-499-143

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                              0.59639



SUM OF PEAK HEIGHTS                6668090.0
SUM OF DE-ISOTOPED PEAKS           6102870.0

DENSITY OF TEST SAMPLE                0.8617

AMOUNT OF RECOVERY                     98.3


AVERAGE MOLECULAR WEIGHT              199.9



                                              *
                                              *  ESTIMATED
                                  VOLUME PCT  *  WEIGHT PCT
                                 ------------ * ------------
   SATURATES                            87.2  *         84.5
      PARAFFINS                  17.3         * 15.3
      NONCOND CYCLOPARAFFINS     30.3         * 28.5
      COND CYCLOPAR 2-RING       25.3         * 25.6
      COND CYCLOPAR 3-RING+      14.1         * 15.0
   AROMATICS                            12.7  *         15.4
    MONO-                          5.9        *       6.4
      BENZENES                    0.6         *  0.6
      NAPHTHENEBENZENES           2.3         *  2.6
      DINAPHTHENEBENZENES         2.9         *  3.1
    DI-                            3.1        *       4.3
      NAPHTHALENES                0.1         *  0.2
      ACENAPHTHENES, DIBENZOFURANS 0.9        *  1.2
      FLUORENES                   2.2         *  2.9
    TRI-                           1.8        *       2.5
      PHENANTHRENES               1.4         *  1.9
      NAPHTHENEPHENANTHRENES      0.3         *  0.5
    TETRA-                         0.3        *       0.5
      PYRENES                     0.3         *  0.5
      CHRYSENES                   0.0         *  0.0
    PENTA-                         0.0        *       0.0
      PERYLENES                   0.0         *  0.0
      DIBENZANTHRACENES           0.0         *  0.0
    THIOPHENO-                     1.1        *       1.5
      BENZOTHIOPHENES             1.0         *  1.3
      DIBENZOTHIOPHENES           0.1         *  0.2
      NAPHTHOBENZOTHIOPHENES      0.0         *  0.0
    UNIDENTIFIED                   0.0        *       0.0
      CLASS I  WITH NAPHPHENAN                *
      CLASS II                    0.0         *  0.0
      CLASS III                   0.0         *  0.0
      CLASS IV                    0.0         *  0.0
      CLASS V                     0.0         *  0.0
      CLASS VI                    0.0         *  0.0
      CLASS VII                   0.0         *  0.0
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MB499145A.MI  06/27/86
1UL MB-499-145

                        MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                 0.59839



SUM OF PEAK HEIGHTS              6334900.0
SUM OF DE-ISOTOPED PEAKS         5825670.0

DENSITY OF TEST SAMPLE               0.8653

AMOUNT OF RECOVERY                  97.1


AVERAGE MOLECULAR WEIGHT           199.9



                                              *
                                              *  ESTIMATED
                                  VOLUME PCT  *  WEIGHT PCT
                                ------------- * ------------
  SATURATES                             87.6  *          84.7
     PARAFFINS                   16.8         * 14.7
     NONCOND CYCLOPARAFFINS      27.6         * 25.8
     COND CYCLOPAR 2-RING        30.9         * 31.0
     COND CYCLOPAR 3-RING+       12.3         * 13.0
  AROMATICS                             12.3  *          15.2
   MONO-                           4.4        *        4.8
     BENZENES                     0.0         *  0.0
     NAPHTHENEBENZENES            1.6         *  1.7
     DINAPHTHENEBENZENES          2.8         *  3.1
   DI-                             3.9        *        4.9
     NAPHTHALENES                 0.3         *  0.3
     ACENAPHTHENES, DBZFURANS     1.2         *  1.5
     FLUORENES                    2.3         *  3.0
   TRI-                            2.2        *        3.1
     PHENANTHRENES                1.7         *  2.3
     NAPHTHENEPHENANTHRENES       0.5         *  0.7
   TETRA--                         0.4        *        0.6
     PYRENES                      0.4         *  0.5
     CHRYSENES                    0.0         *  0.0
   PENTA-                          0.0        *        0.0
     PERYLENES                    0.0         *  0.0
     DIBENZANTHRACENES            0.0         *  0.0
   THIOPHENO-                      1.2        *        1.6
     BENZOTHIOPHENES              1.1         *  1.4
     DIBENZOTHIOPHENES            0.1         *  0.1
     NAPHTHOBENZOTHIOPHENES       0.0         *  0.0
   UNIDENTIFIED                    0.0        *        0.0
     CLASS I  WITH NAPHPHENAN                 *
     CLASS II                     0.0         *  0.0
     CLASS III                    0.0         *  0.0
     CLASS IV                     0.0         *  0.0
     CLASS V                      0.0         *  0.0
     CLASS VI                     0.0         *  0.0
     CLASS VII                    0.0         *  0.0
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MB499145B.MI  06/27/86
1UL MB-499-145

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839



SUM OF PEAK HEIGHTS             6576900.0
SUM OF DE-ISOTOPED PEAKS        6061960.0

DENSITY OF TEST SAMPLE                0.8608

AMOUNT OF RECOVERY                   98.6


AVERAGE MOLECULAR WEIGHT            199.9



                                             *
                                             *  ESTIMATED
                                VOLUME PCT   *  WEIGHT PCT
                               ------------- * ------------
   SATURATES                           89.4  *          86.9
      PARAFFINS                16.6          * 14.6
      NONCOND CYCLOPARAFFINS   31.4          * 29.5
      COND CYCLOPAR 2-RING     26.2          * 26.5
      COND CYCLOPAR 3-RING+    15.0          * 16.1
   AROMATICS                           10.5  *          13.0
    MONO-                          4.0       *      4.4
      BENZENES                  0.0          *  0.0
      NAPHTHENEBENZENES         1.6          *  1.7
      DINAPHTHENEBENZENES       2.4          *  2.6
    DI-                            3.2       *      4.1
      NAPHTHALENES              0.1          *  0.1
      ACENAPHTHENES, DBZFURANS  0.8          *  1.1
      FLUORENES                 2.2          *  2.8
    TRI-                           1.8       *      2.5
      PHENANTHRENES             1.5          *  2.0
      NAPHTHENEPHENANTHRENES    0.3          *  0.5
    TETRA-                         0.3       *      0.5
      PYRENES                   0.3          *  0.5
      CHRYSENES                 0.0          *  0.0
    PENTA-                         0.0       *      0.0
      PERYLENES                 0.0          *  0.0
      DIBENZANTHRACENES         0.0          *  0.0
    THIOPHENO-                     1.0       *      1.3
      BENZOTHIOPHENES           0.8          *  1.1
      DIBENZOTHIOPHENES         0.1          *  0.1
      NAPHTHOBENZOTHIOPHENES    0.0          *  0.0
    UNIDENTIFIED                   0.0       *      0.0
      CLASS I  WITH NAPHPHENAN               *
      CLASS II                  0.0          *  0.0
      CLASS III                 0.0          *  0.0
      CLASS IV                  0.0          *  0.0
      CLASS V                   0.0          *  0.0
      CLASS VI                  0.0          *  0.0
      CLASS VII                 0.0          *  0.0
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MB499145C.MI  06/27/86
1UL MB-499-145

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839



SUM OF PEAK HEIGHTS             6630970.0
SUM OF DE-ISOTOPED PEAKS        6090960.0

DENSITY OF TEST SAMPLE                0.8634

AMOUNT OF RECOVERY                   92.4


AVERAGE MOLECULAR WEIGHT            199.9



                                            *
                                            *  ESTIMATED
                                VOLUME PCT  *  WEIGHT PCT
                               ------------ * ------------
   SATURATES                           86.8 *         83.8
      PARAFFINS                18.3         * 16.1
      NONCOND CYCLOPARAFFINS   30.0         * 28.1
      COND CYCLOPAR 2-RING     24.9         * 25.1
      COND CYCLOPAR 3-RING+    13.3         * 14.2
   AROMATICS                           13.1 *         16.1
    MONO-                           5.2     *      5.6
      BENZENES                  0.0         *  0.0
      NAPHTHENEBENZENES         2.5         *  2.7
      DINAPHTHENEBENZENES       2.7         *  2.9
    DI-                             4.0     *      5.0
      NAPHTHALENES              0.2         *  0.3
      ACENAPHTHENES,DBZFURANS   1.1         *  1.4
      FLUORENES                 2.5         *  3.2
    TRI-                            2.2     *      3.0
      PHENANTHRENES             1.7         *  2.4
      NAPHTHENEPHENANTHRENES    0.4         *  0.6
    TETRA-                          0.5     *      0.7
      PYRENES                   0.4         *  0.7
      CHRYSENES                 0.0         *  0.0
    PENTA-                          0.0     *      0.0
      PERYLENES                 0.0         *  0.0
      DIBENZANTHRACENES         0.0         *  0.0
    THIOPHENO-                      1.1     *      1.5
      BENZOTHIOPHENES           0.9         *  1.2
      DIBENZOTHIOPHENES         0.1         *  0.2
      NAPHTHOBENZOTHIOPHENES    0.0         *  0.0
    UNIDENTIFIED                    0.0     *      0.0
      CLASS I  WITH NAPHPHENAN              *
      CLASS II                  0.0         *  0.0
      CLASS III                 0.0         *  0.0
      CLASS IV                  0.0         *  0.0
      CLASS V                   0.0         *  0.0
      CLASS VI                  0.0         *  0.0
      CLASS VII                 0.0         *  0.0
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MB499178A.MI  06/27/86
1UL MB-499-178

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839



SUM OF PEAK HEIGHTS             7165530.0
SUM OF DE-ISOTOPED PEAKS        6618110.0

DENSITY OF TEST SAMPLE                0.8575

AMOUNT OF RECOVERY                  102.2


AVERAGE MOLECULAR WEIGHT            199.9




                                            *
                                            *  ESTIMATED
                                VOLUME PCT  *  WEIGHT PCT
                               ------------ * ------------
   SATURATES                           89.6 *         87.1
      PARAFFINS                17.7         * 15.7
      NONCOND CYCLOPARAFFINS   31.7         * 29.9
      COND CYCLOPAR 2-RING     26.8         * 27.2
      COND CYCLOPAR 3-RING+    13.2         * 14.2
   AROMATICS                           10.3 *         12.8
    MONO-                           4.3     *      4.7
      BENZENES                  0.0         *  0.0
      NAPHTHENEBENZENES         1.9         *  2.1
      DINAPHTHENEBENZENES       2.3         *  2.6
    DI-                             2.6     *      3.3
      NAPHTHALENES              0.0         *  0.0
      ACENAPHTHENES/DBZFURANS   0.6         *  0.8
      FLUORENES                 1.9         *  2.5
    TRI-                            1.7     *      2.4
      PHENANTHRENES             1.4         *  1.9
      NAPHTHENEPHENANTHRENES    0.3         *  0.4
    TETRA-                          0.3     *      0.4
      PYRENES                   0.2         *  0.4
      CHRYSENES                 0.0         *  0.0
    PENTA-                          0.0     *      0.0
      PERYLENES                 0.0         *  0.0
      DIBENZANTHRACENES         0.0         *  0.0
    THIOPHENO-                      1.2     *      1.7
      BENZOTHIOPHENES           1.1         *  1.5
      DIBENZOTHIOPHENES         0.1         *  0.1
      NAPHTHOBENZOTHIOPHENES    0.0         *  0.0
    UNIDENTIFIED                    0.0     *      0.0
      CLASS I  WITH NAPHPHENAN              *
      CLASS II                  0.0         *  0.0
      CLASS III                 0.0         *  0.0
      CLASS IV                  0.0         *  0.0
      CLASS V                   0.0         *  0.0
      CLASS VI                  0.0         *  0.0
      CLASS VII                 0.0         *  0.0
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64991788.MI  06/27/86
1UL MB-499-178

                            MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                       0.59839



SUM OF PEAK HEIGHTS                 6609540.0
SUM OF DE-ISOTOPED PEAKS            6097300.0

DENSITY OF TEST SAMPLE                 0.8582

AMOUNT OF RECOVERY                    101.4


AVERAGE MOLECULAR WEIGHT              199.9



                                                   *
                                                   *  ESTIMATED
                                      VOLUME PCT   *  WEIGHT PCT
                                     ------------  * ------------
   SATURATES                                89.4  *          86.9
      PARAFFINS                      18.6          * 16.5
      NONCOND CYCLOPARAFFINS         30.2          * 28.5
      COND CYCLOPAR 2-RING           26.6          * 26.9
      COND CYCLOPAR 3-RING+          13.9          * 14.9
   AROMATICS                                10.5  *          13.0
    MONO-                                 4.4      *       4.8
      BENZENES                       0.0           *  0.0
      NAPHTHENEBENZENES              1.9           *  2.1
      DINAPHTHENEBENZENES            2.4           *  2.6
    DI-                                   2.6      *       3.4
      NAPHTHALENES                   0.0           *  0.0
      ACENAPHTHENES, DBZFURANS       0.7           *  0.9
      FLUORENES                      1.9           *  2.5
    TRI-                                  1.7      *       2.4
      PHENANTHRENES                  1.4           *  1.9
      NAPHTHENEPHENANTHRENES         0.3           *  0.5
    TETRA-                                0.3      *       0.5
      PYRENES                        0.3           *  0.4
      CHRYSENES                      0.0           *  0.0
    PENTA-                                0.0      *       0.0
      PERYLENES                      0.0           *  0.0
      DIBENZANTHRACENES              0.0           *  0.0
    THIOPHENO-                            1.3      *       1.7
      BENZOTHIOPHENES                1.1           *  1.5
      DIBENZOTHIOPHENES              0.1           *  0.1
      NAPHTHOBENZOTHIOPHENES         0.0           *  0.0
    UNIDENTIFIED                          0.0      *       0.0
      CLASS I  WITH NAPHPHENAN                     *
      CLASS II                       0.0           *  0.0
      CLASS III                      0.0           *  0.0
      CLASS IV                       0.0           *  0.0
      CLASS V                        0.0           *  0.0
      CLASS VI                       0.0           *  0.0
      CLASS VII                      0.0           *  0.0
```

```
MB499178C.MI  06/27/86
1UL MB-499-178

                        MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  0.59839



SUM OF PEAK HEIGHTS              5925730.0
SUM OF DE-ISOTOPED PEAKS         5442060.0

DENSITY OF TEST SAMPLE              0.8645

AMOUNT OF RECOVERY                 92.9


AVERAGE MOLECULAR WEIGHT          199.9



                                             *
                                             *  ESTIMATED
                                VOLUME PCT   *  WEIGHT PCT
                               ------------- * ------------
   SATURATES                            86.4 *          83.2
     PARAFFINS                  17.9         * 15.8
     NONCOND CYCLOPARAFFINS     31.3         * 29.3
     COND CYCLOPAR 2-RING       23.9         * 24.1
     COND CYCLOPAR 3-RING+      13.1         * 14.0
   AROMATICS                            13.5 *          16.7
    MONO-                           5.1      *      5.5
     BENZENES                    0.1         *  0.1
     NAPHTHENEBENZENES           1.9         *  2.1
     DINAPHTHENEBENZENES         3.0         *  3.2
    DI-                             3.8      *      4.9
     NAPHTHALENES                0.0         *  0.0
     ACENAPHTHENES, DBZFURANS    0.9         *  1.1
     FLUORENES                   2.8         *  3.6
    TRI-                            2.4      *      3.3
     PHENANTHRENES               1.8         *  2.5
     NAPHTHENEPHENANTHRENES      0.5         *  0.7
    TETRA-                          0.4      *      0.6
     PYRENES                     0.3         *  0.5
     CHRYSENES                   0.0         *  0.0
    PENTA-                          0.0      *      0.0
     PERYLENES                   0.0         *  0.0
     DIBENZANTHRACENES           0.0         *  0.0
    THIOPHENO-                      1.6      *      2.2
     BENZOTHIOPHENES             1.4         *  1.8
     DIBENZOTHIOPHENES           0.2         *  0.3
     NAPHTHOBENZOTHIOPHENES      0.0         *  0.0
    UNIDENTIFIED                    0.0      *      0.0
     CLASS I  WITH NAPHPHENAN                *
     CLASS II                    0.0         *  0.0
     CLASS III                   0.0         *  0.0
     CLASS IV                    0.0         *  0.0
     CLASS V                     0.0         *  0.0
     CLASS VI                    0.0         *  0.0
     CLASS VII                   0.0         *  0.0
```

```
MB1410701A.MI  07/01/86
1UL MB 499-141

                   MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                              0 59839


SUM OF PEAK HEIGHTS                27333400.0
SUM OF DE-ISOTOPED PEAKS           25213300.0

DENSITY OF TEST SAMPLE                  0.8602

AMOUNT OF RECOVERY                     78.4


AVERAGE MOLECULAR WEIGHT              199.9



                                                 *
                                                 *  ESTIMATED
                                     VOLUME PCT  *  WEIGHT PCT
                                    ------------ * ------------
   SATURATES                                88.5 *          85.5
      PARAFFINS                     17.9         * 15.8
      NONCOND CYCLOPARAFFINS        35.2         * 33.1
      COND CYCLOPAR 2-RING          23.6         * 23.9
      COND CYCLOPAR 3-RING+         11.7         * 12.5
   AROMATICS                                11.4 *          14.4
    MONO-                                2.5     *       2.8
      BENZENES                       0.0         *  0.0
      NAPHTHENEBENZENES              0.7         *  0.7
      DINAPHTHENEBENZENES            1.8         *  2.0
    DI-                                  5.0     *       6.4
      NAPHTHALENES                   0.3         *  0.4
      ACENAPHTHENES, DBZFURANS       1.4         *  1.7
      FLUORENES                      3.3         *  4.2
    TRI-                                 2.5     *       3.5
      PHENANTHRENES                  2.2         *  3.0
      NAPHTHENEPHENANTHRENES         0.3         *  0.4
    TETRA-                               0.4     *       0.5
      PYRENES                        0.4         *  0.5
      CHRYSENES                      0.0         *  0.0
    PENTA-                               0.0     *       0.0
      PERYLENES                      0.0         *  0.0
      DIBENZANTHRACENES              0.0         *  0.0
    THIOPHENO-                           0.8     *       1.0
      BENZOTHIOPHENES                0.6         *  0.8
      DIBENZOTHIOPHENES              0.1         *  0.2
      NAPHTHOBENZOTHIOPHENES         0.0         *  0.0
    UNIDENTIFIED                         0.0     *       0.0
      CLASS I  WITH NAPHPHENAN                   *
      CLASS II                       0.0         *  0.0
      CLASS III                      0.0         *  0.0
      CLASS IV                       0.0         *  0.0
      CLASS V                        0.0         *  0.0
      CLASS VI                       0.0         *  0.0
      CLASS VII                      0.0         *  0.0
```

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MB14107018. MI   07/01/86
1UL MB 499-141

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                               0. 59839


SUM OF PEAK HEIGHTS                 24911700. 0
SUM OF DE-ISOTOPED PEAKS            22980800. 0

DENSITY OF TEST SAMPLE                   0. 8598

AMOUNT OF RECOVERY                     78. 5


AVERAGE MOLECULAR WEIGHT               199. 9


                                                 *
                                                 *  ESTIMATED
                                    VOLUME PCT   *  WEIGHT PCT
                                    ------------ * ------------
    SATURATES                              88. 4 *          85. 3
       PARAFFINS                    15. 0        * 15. 9
       NONCOND CYCLOPARAFFINS       33. 3        * 33. 2
       COND CYCLOPAR 2-RING         23. 3        * 23. 6
       COND CYCLOPAR 3-RING+        11. 6        * 12. 4
    AROMATICS                              11. 5 *          14. 6
     MONO-                              2. 7     *      3. 0
       BENZENES                      0. 0        *  0. 0
       NAPHTHENEBENZENES             0. 8        *  0. 9
       DINAPHTHENEBENZENES           1. 8        *  2. 0
     DI-                                5. 0     *      6. 4
       NAPHTHALENES                  0. 2        *  0. 3
       ACENAPHTHENES, DBZFURANS      1. 3        *  1. 7
       FLUORENES                     3. 3        *  4. 3
     TRI-                               2. 5     *      3. 5
       PHENANTHRENES                 2. 2        *  3. 1
       NAPHTHENEPHENANTHRENES        0. 3        *  0. 4
     TETRA-                             0. 3     *      0. 4
       PYRENES                       0. 3        *  0. 4
       CHRYSENES                     0. 0        *  0. 0
     PENTA-                             0. 0     *      0. 0
       PERYLENES                     0. 0        *  0. 0
       DIBENZANTHRACENES             0. 0        *  0. 0
     THIOPHENO-                         0. 8     *      1. 1
       BENZOTHIOPHENES               0. 6        *  0. 8
       DIBENZOTHIOPHENES             0. 1        *  0. 2
       NAPHTHOBENZOTHIOPHENES        0. 0        *  0. 0
     UNIDENTIFIED                       0. 0     *      0. 0
       CLASS I  WITH NAPHPHENAN                  *
       CLASS II                      0. 0        *  0. 0
       CLASS III                     0. 0        *  0. 0
       CLASS IV                      0. 0        *  0. 0
       CLASS V                       0. 0        *  0. 0
       CLASS VI                      0. 0        *  0. 0
       CLASS VII                     0. 0        *  0. 0
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MB1410701C.MI  07/01/86
1UL MB 499-141

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839


SUM OF PEAK HEIGHTS            24063100.0
SUM OF DE-ISOTOPED PEAKS       22202200.0

DENSITY OF TEST SAMPLE                0.8597

AMOUNT OF RECOVERY                   79.0


AVERAGE MOLECULAR WEIGHT            199.9



                                            *
                                            *  ESTIMATED
                                VOLUME PCT  *  WEIGHT PCT
                               ------------ * ------------
   SATURATES                           88.5 *         85.4
      PARAFFINS                18.0         * 15.9
      NONCOND CYCLOPARAFFINS   35.0         * 33.0
      COND CYCLOPAR 2-RING     23.7         * 24.0
      COND CYCLOPAR 3-RING+    11.6         * 12.4
   AROMATICS                           11.4 *         14.5
    MONO-                          2.7      *      3.0
      BENZENES                  0.0         *  0.0
      NAPHTHENEBENZENES         0.8         *  0.9
      DINAPHTHENEBENZENES       1.9         *  2.1
    DI-                            4.9      *      6.2
      NAPHTHALENES              0.2         *  0.2
      ACENAPHTHENES, DBZFURANS  1.3         *  1.6
      FLUORENES                 3.3         *  4.2
    TRI-                           2.5      *      3.5
      PHENANTHRENES             2.2         *  3.0
      NAPHTHENEPHENANTHRENES    0.3         *  0.4
    TETRA-                         0.2      *      0.4
      PYRENES                   0.2         *  0.4
      CHRYSENES                 0.0         *  0.0
    PENTA-                         0.0      *      0.0
      PERYLENES                 0.0         *  0.0
      DIBENZANTHRACENES         0.0         *  0.0
    THIOPHENO-                     0.9      *      1.2
      BENZOTHIOPHENES           0.6         *  0.9
      DIBENZOTHIOPHENES         0.2         *  0.3
      NAPHTHOBENZOTHIOPHENES    0.0         *  0.0
    UNIDENTIFIED                   0.0      *      0.0
     CLASS I  WITH NAPHPHENAN               *
     CLASS II                   0.0         *  0.0
     CLASS III                  0.0         *  0.0
     CLASS IV                   0.0         *  0.0
     CLASS V                    0.0         *  0.0
     CLASS VI                   0.0         *  0.0
     CLASS VII                  0.0         *  0.0
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MB1430701A.RI  07/01/86
1UL MB 499-143

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839



SUM OF PEAK HEIGHTS           32779300.0
SUM OF DE-ISOTOPED PEAKS      30118300.0

DENSITY OF TEST SAMPLE                0.8671

AMOUNT OF RECOVERY                   80.3


AVERAGE MOLECULAR WEIGHT            1 7.9



                                             *
                                             *  ESTIMATED
                                VOLUME PCT   *  WEIGHT PCT
                               ------------  * ------------
   SATURATES                           84.2  *         80.7
      PARAFFINS                16.9          * 14.8
      NONCOND CYCLOPARAFFINS   32.9          * 30.7
      COND CYCLOPAR 2-RING     22.3          * 22.4
      COND CYCLOPAR 3-RING+    11.9          * 12.6
   AROMATICS                           15.7  *         19.2
    MONO-                          6.2       *      6.7
      BENZENES                  0.5          *  0.5
      NAPHTHENEBENZENES         2.2          *  2.4
      DINAPHTHENEBENZENES       3.5          *  3.8
    DI-                            4.6       *      5.8
      NAPHTHALENES              0.1          *  0.2
      ACENAPHTHENES, DBZFURANS  1.3          *  1.6
      FLUORENES                 3.0          *  3.9
    TRI-                           2.7       *      3.7
      PHENANTHRENES             2.0          *  2.8
      NAPHTHENEPHENANTHRENES    0.6          *  0.9
    TETRA-                         0.4       *      0.6
      PYRENES                   0.4          *  0.6
      CHRYSENES                 0.0          *  0.0
    PENTA-                         0.0       *      0.0
      PERYLENES                 0.0          *  0.0
      DIBENZANTHRACENES         0.0          *  0.0
    THIOPHENO-                     1.6       *      2.2
      BENZOTHIOPHENES           1.4          *  1.8
      DIBENZOTHIOPHENES         0.2          *  0.3
      NAPHTHOBENZOTHIOPHENES    0.0          *  0.0
    UNIDENTIFIED                   0.0       *      0.0
      CLASS I  WITH NAPHPHENAN               *
      CLASS II                  0.0          *  0.0
      CLASS III                 0.0          *  0.0
      CLASS IV                  0.0          *  0.0
      CLASS V                   0.0          *  0.0
      CLASS VI                  0.0          *  0.0
      CLASS VII                 0.0          *  0.0
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MB1430701B. MI  07/01/86
1UL MB 499-143

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                   0. 59839



SUM OF PEAK HEIGHTS               27171800. 0
SUM OF DE-ISOTOPED PEAKS          24969900. 0

DENSITY OF TEST SAMPLE                 0. 8680

AMOUNT OF RECOVERY                    78. 8


AVERAGE MOLECULAR WEIGHT             199. 9



                                                *
                                                *  ESTIMATED
                                    VOLUME PCT  *  WEIGHT PCT
                                   ------------ * ------------
  SATURATES                                83. 9 *           80. 4
     PARAFFINS                     16. 2         * 14. 2
     NONCOND CYCLOPARAFFINS        33. 4         * 31. 2
     COND CYCLOPAR 2-RING          22. 3         * 22. 3
     COND CYCLOPAR 3-RING+         11. 8         * 12. 5
  AROMATICS                                16. 0 *           19. 5
   MONO-                                 6. 5    *        6. 9
     BENZENES                       0. 4         *  0. 4
     NAPHTHENEBENZENES              2. 3         *  2. 4
     DINAPHTHENEBENZENES            3. 7         *  4. 0
   DI-                                   4. 5    *        5. 8
     NAPHTHALENES                   0. 1         *  0. 1
     ACENAPHTHENES, DBZFURANS       1. 2         *  1. 5
     FLUORENES                      3. 1         *  4. 0
   TRI-                                  2. 9    *        4. 0
     PHENANTHRENES                  2. 3         *  3. 1
     NAPHTHENEPHENANTHRENES         0. 5         *  0. 8
   TETRA-                                0. 4    *        0. 6
     PYRENES                        0. 4         *  0. 6
     CHRYSENES                      0. 0         *  0. 0
   PENTA-                                0. 0    *        0. 0
MB1430701C. MI  07/01/86
1UL MB 499-143

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                   0. 59839



SUM OF PEAK HEIGHTS               32267700. 0
SUM OF DE-ISOTOPED PEAKS          29676700. 0

DENSITY OF TEST SAMPLE                 0. 8665

AMOUNT OF RECOVERY                    79. 9


AVERAGE MOLECULAR WEIGHT             199. 9
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                                         *
                                         *  ESTIMATED
                             VOLUME PCT  *  WEIGHT PCT
                            ------------ * ------------
SATURATES                          84. 1 *        80. 7
   PARAFFINS                17. 0        * 14. 9
   NONCOND CYCLOPARAFFINS   33. 4        * 31. 2
   COND CYCLOPAR 2-RING     21. 9        * 22. 0
   COND CYCLOPAR 3-RING+    11. 7        * 12. 4
AROMATICS                          15. 8 *        19. 2
 MONO-                          6. 4     *     6. 9
   BENZENES                  0. 4        *  0. 4
   NAPHTHENEBENZENES         2. 1        *  2. 3
   DINAPHTHENEBENZENES       3. 7        *  4. 0
 DI-                            4. 5     *     5. 7
   NAPHTHALENES              0. 1        *  0. 1
   ACENAPHTHENES, DBZFURANS  1. 2        *  1. 5
   FLUORENES                 3. 1        *  4. 0
 TRI-                           2. 6     *     3. 5
   PHENANTHRENES             2. 0        *  2. 7
   NAPHTHENEPHENANTHRENES    0. 5        *  0. 8
 TETRA-                         0. 4     *     0. 6
   PYRENES                   0. 4        *  0. 6
   CHRYSENES                 0. 0        *  0. 0
 PENTA-                         0. 0     *     0. 0
   PERYLENES                 0. 0        *  0. 0
   DIBENZANTHRACENES         0. 0        *  0. 0
 THIOPHENO-                     1. 8     *     2. 4
   BENZOTHIOPHENES           1. 5        *  2. 0
   DIBENZOTHIOPHENES         0. 1        *  0. 1
   NAPHTHOBENZOTHIOPHENES    0. 0        *  0. 1
 UNIDENTIFIED                   0. 0     *     0. 0
   CLASS I  WITH NAPHPHENAN              *
   CLASS II                  0. 0        *  0. 0
   CLASS III                 0. 0        *  0. 0
   CLASS IV                  0. 0        *  0. 0
   CLASS V                   0. 0        *  0. 0
   CLASS VI                  0. 0        *  0. 0
   CLASS VII                 0. 0        *  0. 0
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MB1450701A.MI  07/01/86
1UL MB 499-145

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0. 59839



SUM OF PEAK HEIGHTS            30588400. 0
SUM OF DE-ISOTOPED PEAKS       28164500. 0

DENSITY OF TEST SAMPLE                0. 8652

AMOUNT OF RECOVERY                   78. 7


AVERAGE MOLECULAR WEIGHT            199. 9



                                            *
                                            *  ESTIMATED
                                VOLUME PCT  *  WEIGHT PCT
                               ------------ * ------------
   SATURATES                           86. 1 *         82. 8
      PARAFFINS                16. 8        * 14. 8
      NONCOND CYCLOPARAFFINS   34. 2        * 32. 0
      COND CYCLOPAR 2-RING     22. 8        * 23. 0
      COND CYCLOPAR 3-RING+    12. 1        * 12. 9
   AROMATICS                           13. 8 *         17. 1
    MONO-                           4. 4    *      4. 7
      BENZENES                  0. 0        *  0. 0
      NAPHTHENEBENZENES         1. 5        *  1. 7
      DINAPHTHENEBENZENES       2. 3        *  3. 0
    DI-                             4. 8    *      6. 0
      NAPHTHALENES              0. 2        *  0. 3
      ACENAPHTHENES, DBZFURANS  1. 2        *  1. 5
      FLUORENES                 3. 2        *  4. 1
    TRI-                            2. 7    *      3. 7
      PHENANTHRENES             2. 1        *  2. 9
      NAPHTHENEPHENANTHRENES    0. 5        *  0. 8
    TETRA-                          0. 4    *      0. 6
      PYRENES                   0. 4        *  0. 6
      CHRYSENES                 0. 0        *  0. 0
    PENTA-                          0. 0    *      0. 0
      PERYLENES                 0. 0        *  0. 0
      DIBENZANTHRACENES         0. 0        *  0. 0
    THIOPHENO-                      1. 4    *      1. 8
      BENZOTHIOPHENES           1. 2        *  1. 6
      DIBENZOTHIOPHENES         0. 0        *  0. 1
      NAPHTHOBENZOTHIOPHENES    0. 0        *  0. 0
    UNIDENTIFIED                    0. 0    *      0. 0
      CLASS I  WITH NAPHPHENAN              *
      CLASS II                  0. 0        *  0. 0
      CLASS III                 0. 0        *  0. 0
      CLASS IV                  0. 0        *  0. 0
      CLASS V                   0. 0        *  0. 0
      CLASS VI                  0. 0        *  0. 0
      CLASS VII                 0. 0        *  0. 0
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MB14507018.MI  07/01/86
1UL MB 499-145

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0.59839


SUM OF PEAK HEIGHTS            31316300.0
SUM OF DE-ISOTOPED PEAKS       28796500.0

DENSITY OF TEST SAMPLE                0.8658

AMOUNT OF RECOVERY                   78.8


AVERAGE MOLECULAR WEIGHT            199.9


                                            *
                                            *  ESTIMATED
                                VOLUME PCT  *  WEIGHT PCT
                               ------------ * ------------
   SATURATES                           86.1 *         82.8
      PARAFFINS                17.0         * 14.9
      NONCOND CYCLOPARAFFINS   33.5         * 31.4
      COND CYCLOPAR 2-RING     23.2         * 23.3
      COND CYCLOPAR 3-RING+    12.3         * 13.0
   AROMATICS                           13.8 *         17.1
    MONO-                           4.4     *      4.8
      BENZENES                  0.0         *  0.0
      NAPHTHENEBENZENES         1.5         *  1.7
      DINAPHTHENEBENZENES       2.8         *  3.0
    DI-                             4.5     *      5.7
      NAPHTHALENES              0.1         *  0.1
      ACENAPHTHENES.DBZFURANS   1.2         *  1.5
      FLUORENES                 3.1         *  4.1
    TRI-                            2.7     *      3.8
      PHENANTHRENES             2.1         *  2.9
      NAPHTHENEPHENANTHRENES    0.5         *  0.8
    TETRA-                          0.4     *      0.6
      PYRENES                   0.4         *  0.6
      CHRYSENES                 0.0         *  0.0
    PENTA-                          0.0     *      0.0
      PERYLENES                 0.0         *  0.0
      DIBENZANTHRACENES         0.0         *  0.0
    THIOPHENO-                      1.5     *      2.1
      BENZOTHIOPHENES           1.2         *  1.6
      DIBENZOTHIOPHENES         0.2         *  0.4
      NAPHTHOBENZOTHIOPHENES    0.0         *  0.0
    UNIDENTIFIED                    0.0     *      0.0
      CLASS I  WITH NAPHPHENAN              *
      CLASS II                  0.0         *  0.0
      CLASS III                 0.0         *  0.0
      CLASS IV                  0.0         *  0.0
      CLASS V                   0.0         *  0.0
      CLASS VI                  0.0         *  0.0
      CLASS VII                 0.0         *  0.0
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MB1450701C. MI  07/01/86
1UL MB 499-143

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                            0. 59839


SUM OF PEAK HEIGHTS           28965800. 0
SUM OF DE-ISOTOPED PEAKS      26675100. 0

DENSITY OF TEST SAMPLE               0. 8662

AMOUNT OF RECOVERY                  77. 9


AVERAGE MOLECULAR WEIGHT           199. 9



                                           *
                                           *  ESTIMATED
                               VOLUME PCT  *  WEIGHT PCT
                              ------------ * ------------
   SATURATES                         85. 8 *         82. 4
      PARAFFINS               16. 9        * 14. 8
      NONCOND CYCLOPARAFFINS  33. 3        * 31. 1
      COND CYCLOPAR 2-RING    23. 5        * 23. 6
      COND CYCLOPAR 3-RING+   12. 0        * 12. 8
   AROMATICS                         14. 1 *         17. 5
    MONO-                          4. 4    *       4. 8
      BENZENES                 0. 0        *  0. 0
      NAPHTHENEBENZENES        1. 6        *  1. 7
      DINAPHTHENEBENZENES      2. 8        *  3. 1
    DI-                            4. 9    *       6. 3
      NAPHTHALENES             0. 2        *  0. 2
      ACENAPHTHENES, DBZFURANS 1. 4        *  1. 8
      FLUORENES                3. 2        *  4. 2
    TRI-                           2. 8    *       3. 9
      PHENANTHRENES            2. 2        *  3. 1
      NAPHTHENEPHENANTHRENES   0. 5        *  0. 7
    TETRA-                         0. 4    *       0. 6
      PYRENES                  0. 4        *  0. 6
      CHRYSENES                0. 0        *  0. 0
    PENTA-                         0. 0    *       0. 0
      PERYLENES                0. 0        *  0. 0
      DIBENZANTHRACENES        0. 0        *  0. 0
    THIOPHENO-                     1. 3    *       1. 8
      BENZOTHIOPHENES          1. 2        *  1. 6
      DIBENZOTHIOPHENES        0. 1        *  0. 1
      NAPHTHOBENZOTHIOPHENES   0. 0        *  0. 0
    UNIDENTIFIED                   0. 0    *       0. 0
     CLASS I  WITH NAPHPHENAN              *
     CLASS II                  0. 0        *  0. 0
     CLASS III                 0. 0        *  0. 0
     CLASS IV                  0. 0        *  0. 0
     CLASS V                   0. 0        *  0. 0
     CLASS VI                  0. 0        *  0. 0
     CLASS VII                 0. 0        *  0. 0
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MB17807016 01   /01/85
VOL MS 499-174

                         MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                      0. 59839



SUM OF PEAK HEIGHTS                   28138300. 0
SUM OF DE-ISOTOPED PEAKS              25907100. 0

DENSITY OF TEST SAMPLE                      0. 8651

AMOUNT OF RECOVERY                         90. 4


AVERAGE MOLECULAR WEIGHT                  199. 9




                                                   *
                                                   *  ESTIMATED
                                       VOLUME PCT  *  WEIGHT PCT
                                      ------------ *  ------------
   SATURATES                                85. 5  *           82. 2
      PARAFFINS                       16. 5        * 14. 5
      NONCOND CYCLOPARAFFINS          34. 5        * 32. 3
      COND CYCLOPAR 2-RING            22. 1        * 22. 2
      COND CYCLOPAR 3-RING+           12. 3        * 13. 0
   AROMATICS                                14. 4  *           17. 7
    MONO-                                 5. 3     *        5. 8
      BENZENES                         0. 2        *  0. 2
      NAPHTHENEBENZENES                1. 9        *  2. 1
      DINAPHTHENOBENZENES              3. 1        *  3. 3
    DI-                                   4. 2     *        5. 5
      NAPHTHALENES                     0. 1        *  0. 1
      ACENAPHTHENES&DIBENZOFURANS      1. 0        *  1. 3
      FLUORENES                        3. 1        *  4. 0
    TRI-                                  2. 5     *        3. 6
      PHENANTHRENES                    2. 0        *  2. 8
      NAPHTHENOPHENANTHRENES           0. 5        *  0. 8
    TETRA-                                0. 3     *        0. 5
      PYRENES                          0. 3        *  0. 5
      CHRYSENES                        0. 0        *  0. 0
    PENTA-                                0. 0     *        0. 0
      PERYLENES                        0. 0        *  0. 0
      DIBENZANTHRACENES                0. 0        *  0. 0
    THIOPHENO-                            1. 6     *        2. 1
      BENZOTHIOPHENES                  1. 5        *  1. 9
      DIBENZOTHIOPHENES                0. 1        *  0. 2
      NAPHTHOBENZOTHIOPHENES           0. 0        *  0. 0
    UNIDENTIFIED                          0. 0     *        0. 0
      CLASS I  WITH NAPHPHENAN                     *
      CLASS II                         0. 0        *  0. 0
      CLASS III                        0. 0        *  0. 0
      CLASS IV                         0. 0        *  0. 0
      CLASS V                          0. 0        *  0. 0
      CLASS VI                         0. 0        *  0. 0
      CLASS VII                        0. 0        *  0. 0
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MB1/807016.MI  07/01/80
1UL MB 179-178

                          MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                                  0 59839



SUM OF PEAK HEIGHTS                28439800 0
SUM OF DE-ISOTOPED PEAKS           26198100. 0

DENSITY OF TEST SAMPLE                  0. 8648

AMOUNT OF RECOVERY                     80. 9


AVERAGE MOLECULAR WEIGHT              199. 9



                                                 *
                                                 *  ESTIMATED
                                   VOLUME PCT    *  WEIGHT PCT
                                  ------------   * ------------
   SATURATES                                85. 8 *           82. 6
      PARAFFINS                    16. 2          * 14. 2
      NONCOND CYCLOPARAFFINS       34. 5          * 32. 4
      COND CYCLOPAR 2-RING         22. 6          * 20. 4
      COND CYCLOPAR 3-RING+        12. 5          * 13. 3
   AROMATTCS                                14. 1 *           17. 3
    MONO-                               5. 3      *       5. 8
      BENZENES                      0. 4          *  0. 4
      NAPHTHENEBENZENES             1. 9          *  2. 0
      DINAPHTHENEBENZENES           3. 0          *  3. 3
    DI-                                 4. 2      *       5. 3
      NAPHTHALENES                  0. 0          *  0. 0
      ACENAPHTHENES, DBZFURANS      1. 1          *  1. 4
      FLUORENES                     3. 0          *  3. 8
    TRI-                                2. 5      *       3. 4
      PHENANTHRENES                 1. 9          *  2. 7
      NAPHTHENEPHENANTHRENES        0. 5          *  0. 7
    TETRA-                              0. 4      *       0. 6
      PYRENES                       0. 4          *  0. 6
      CHRYSENES                     0. 0          *  0. 0
    PENTA-                              0. 0      *       0. 0
      PERYLENES                     0. 0          *  0. 0
      DIBENZANTHRACENES             0. 0          *  0. 0
    THIOPHENO-                          1. 5      *       2. 0
      BENZOTHIOPHENES               1. 3          *  1. 8
      DIBENZOTHIOPHENES             0. 1          *  0. 2
      NAPHTHOBENZOTHIOPHENES        0. 0          *  0. 0
    UNIDENTIFIED                        0. 0      *       0. 0
      CLASS I  WITH NAPHPHENAN                    *
      CLASS II                      0. 0          *  0. 0
      CLASS III                     0. 0          *  0. 0
      CLASS IV                      0. 0          *  0. 0
      CLASS V                       0. 0          *  0. 0
      CLASS VI                      0. 0          *  0. 0
      CLASS VII                     0. 0          *  0. 0
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MB17S0701C MI  07/01/85
1UL MB 499-178

                    MASS SPECTRAL ANALYSIS OF PETROLEUM OILS
AIN FACTOR                              0.59839


SUM OF PEAK HEIGHTS              29021500.0
SUM OF DE-ISOTOPED PEAKS         26713800.0

DENSITY OF TEST SAMPLE                  0.8659

AMOUNT OF RECOVERY                     80.3


AVERAGE MOLECULAR WEIGHT              199.9


                                                *
                                                *  ESTIMATED
                                    VOLUME PCT  *  WEIGHT PCT
                                   ------------ * ------------
   SATURATES                              85.6  *          82.3
      PARAFFINS                     15.8        * 13.9
      NONCOND CYCLOPARAFFINS        34.8        * 32.5
      COND CYCLOPAR 2-RING          22.5        * 22.6
      COND CYCLOPAR 3-RING+         12.3        * 13.1
   AROMATICS                              14.3  *          17.6
    MONO-                              5.2      *       5.6
      BENZENES                       0.2        *  0.2
      NAPHTHENEBENZENES              1.9        *  2.1
      DINAPHTHENEBENZENES            3.0        *  3.3
    DI-                                4.3      *       5.5
      NAPHTHALENES                   0.1        *  0.1
      ACENAPHTHENES, DBZFURANS       1.0        *  1.3
      FLUORENES                      3.1        *  4.0
    TRI-                               2.5      *       3.5
      PHENANTHRENES                  2.0        *  2.7
      NAPHTHENEPHENANTHRENES         0.5        *  0.7
    TETRA-                             0.4      *       0.6
      PYRENES                        0.4        *  0.6
      CHRYSENES                      0.0        *  0.0
    PENTA-                             0.0      *       0.0
      PERYLENES                      0.0        *  0.0
      DIBENZANTHRACENES              0 0        *  0.0
    THIOPHENO-                         1.7      *       2.2
      BENZOTHIOPHENES                1.4        *  1.7
      DIBENZOTHIOPHENES              0.1        *  0.1
      NAPHTHOBENZOTHIOPHENES         0.2        *  0.1
    UNIDENTIFIED                       0.0      *       0.0
      CLASS [illegible]                         *
      CLASS II                       0.0        *  0.0
      CLASS III                      0.0        *  0.0
      CLASS IV                       0.0        *  0.0
      CLASS V                        0.0        *  0.0
      CLASS VI                       0.0        *  0.0
      CLASS VII                      0.0        *  0.0
```